Intra- and Intermolecular C-H Activation by Bis(phenolate)pyridineiridium(III) Complexes

Ross Fu, John E. Bercaw, and Jay A. Labinger**

Supporting Information

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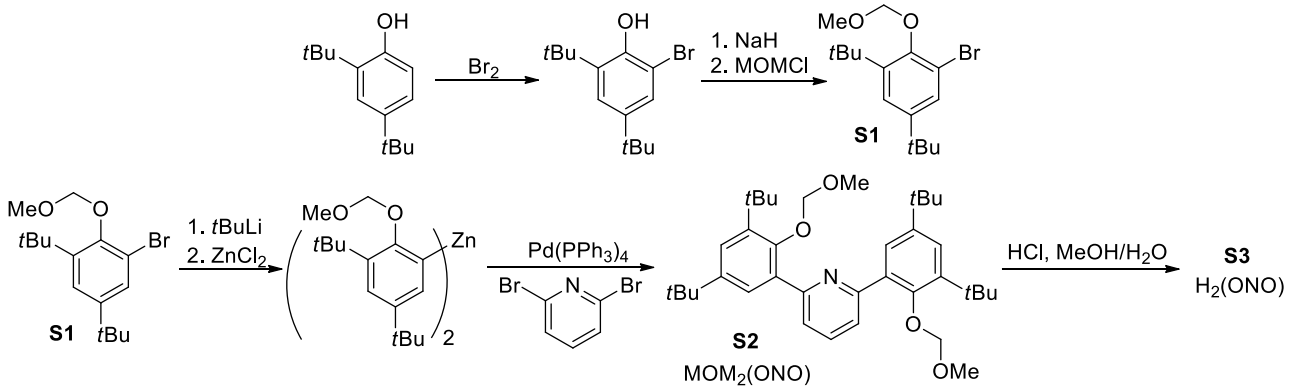
I. Synthesis of the ligand H_2(ONO) (S3)

The synthesis, which closely follows a previously reported procedure,[1] is outlined in Scheme S1.



Scheme S1

Synthesis of *O*-methoxymethyl-2,4-di-*tert*-butyl-6-bromophenoxide, S1. Bromine (3.7 mL, 12 g, 73 mmol) was added via syringe to a solution of 2,4-di-*tert*-butylphenol (15 g, 73 mmol) in CH_2Cl_2 (200 mL). The brown color of Br_2 disappeared upon addition. GC-MS analysis after 5 min shows only the presence of the desired brominated product (M^+ = 284 and 286). The organic mixture was washed with water, then dried over $MgSO_4$, and filtered. Removal of volatile material by rotary evaporation gave a golden oil which solidified after placing under high vacuum (<1 mTorr). This material (4,6-di-t-butyl-2-bromophenol) was dissolved in dry THF (200 mL) under argon, and was deprotonated with NaH (1.92 g, 80 mmol). After the addition of NaH the reaction mixture was stirred for 1 h at room temperature, then MOMCl (6.1 mL, 6.5 g, 80 mmol) was added via syringe. The reaction mixture was stirred at room temperature for 9 h. Water was added and the mixture was concentrated under vacuum. The desired product was extracted with CH_2Cl_2 (three times); the combined organic fractions were dried over $MgSO_4$, filtered, and dried under high vacuum overnight to give 23.5 g (98% yield over two steps) of **S1** as a golden oil. ^{1}H-NMR (300 MHz, $CDCl_3$) δ = 1.30 (s, 9H, $C(CH_3)_3$), 1.44 (s, 9H, $C(CH_3)_3$), 3.70 (s, 3H, OCH_3), 5.23 (s, 2H, OCH_2O), 7.32 (d, 2H, aryl-H), 7.41 (d, 2H, aryl-H). ^{13}C-NMR (75 MHz, $CDCl_3$) δ = 31.0 ($C(CH_3)_3$), 31.5 ($C(CH_3)_3$), 34.8 ($C(CH_3)_3$), 36.1 ($C(CH_3)_3$), 57.9 (OCH_3), 99.5 (OCH_2O), 117.7, 124.1, 128.9, 144.6, 147.8, 150.7 (aryl). GC-MS: M^+ = 328.

Synthesis of MOM_2(ONO), S2. A mixture of **S1** (5.19 g, 15.8 mmol) and THF (25 mL) in a Schlenk tube fitted with a screw-in Teflon stopper was frozen in a cold well, along with a solution of *t*BuLi (2.13 g, 33.3 mmol, 2.1 eq) in hexanes (10 mL), in an inert atmosphere glove box. Both solutions were taken out of the box, and the *t*BuLi solution was added to the solution of **S1** while allowing the latter to thaw. The mixture was stirred for 1 h while allowing it to reach room temperature. $ZnCl_2$ (1.51 g, 7.12 mmol, 0.70 eq) was added with the aid of THF. After stirring the reaction mixture for 30 minutes, 1,3-dibromobenzene (1.69 g, 7.12 mmol, 0.45 eq) and $Pd(PPh_3)_4$ (188.4 mg, 0.163 mmol, 0.01 eq) were added with the aid of some THF. The reaction vessel was placed in an oil bath preheated to 75 °C and stirred for 16 h, then allowed to cool to room temperature and quenched with water. Volatile materials

were removed under vacuum and water was added. This mixture was extracted with Et_2O (three times). The combined organics were dried over $MgSO_4$, filtered, and concentrated by rotary evaporation. The resulting residue was suspended in MeOH and cooled to -25 °C. The resulting white precipitate was collected by filtration through a sintered glass funnel, washed with cold MeOH, and immediately used for the synthesis of **S3**. ^{1}H-NMR (300 MHz, $CDCl_3$) δ = 1.37 (s, 18H, $C(CH_3)_3$), 1.51 (s, 18H, $C(CH_3)_3$), 3.41 (s, 6H, OCH_3), 4.64 (s, 4H, OCH_2O), 7.45 (d, 2H, aryl-H), 7.61 (d, 2H, aryl-H), 7.68-7.80 (m, 3H, NC_5H_3). ^{13}C-NMR (75 MHz, $CDCl_3$) δ = 31.1 ($C(CH_3)_3$), 31.6 ($C(CH_3)_3$), 34.8 ($C(CH_3)_3$), 35.6 ($C(CH_3)_3$), 57.6 (OCH_3), 99.7 (OCH_2O), 123.2, 125.2, 126.7, 134.1, 136.1, 142.5, 146.1, 151.5, 158.4 (aryl).

Synthesis of H_2(ONO), S3. Compound **S2** was suspended in 25 mL of MeOH, and 25 mL of concentrated HCl was added. This mixture was heated at 80 °C for 5 h. After cooling, volatile materials were removed under vacuum yielding 3.45 g (0.70 mmol, 90% based on **S1**) of **S3** as a white powder. ^{1}H-NMR (300 MHz, $CDCl_3$) δ = 1.39 (s, 18H, $C(CH_3)_3$), 1.48 (s, 18H, $C(CH_3)_3$), 7.46 (d, 2H, aryl-H), 7.51 (d, 2H, aryl-H), 7.67 (d, 2H, 3,5-NC_5H-H_2), 8.01 (t, 1H, 4-NC_5H_2-H), 10.59 (s, 2H, OH). ^{13}C-NMR (75 MHz, $CDCl_3$) δ = 29.8 ($C(CH_3)_3$), 31.8 ($C(CH_3)_3$), 34.6 ($C(CH_3)_3$), 35.6 ($C(CH_3)_3$), 120.5, 121.3, 123.0, 126.4, 137.5, 140.0, 141.5, 153.3, 157.6 (aryl). HRMS $C_{33}H_{45}O_2N$: Calculated: 487.3450. Measured: 487.3446.

II. Kinetics Results

1. KIE for intramolecular C-H activation.

The k_{obs} determined for conversion of (ONO$^{t\text{Bu}}$)Ir[P(C_6D_5)$_3$]$_2$Me (**12**-d_{30}) to **17**-d_{36} in C_6D_6 (Figure S1) was 4.4(6) x 10^{-5} s^{-1}, which in combination with the value for the all-protio analog (Figure 8, main text) gives KIE = 4(1).

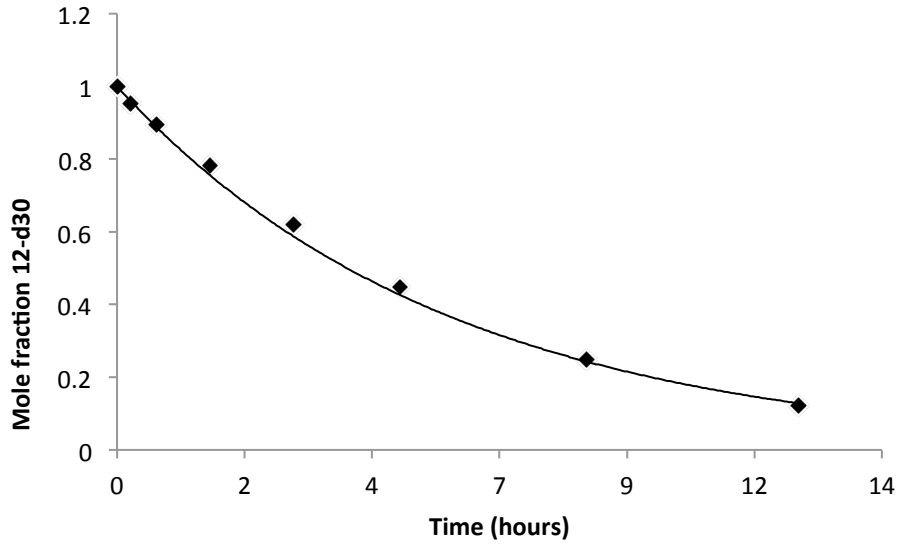


Figure S1. Conversion of **12**-d_{30} to **17**-d_{36} in C_6D_6.

2. Effect of added triphenylphosphine on rate of conversion of **12** to **17**.

The data used to construct Figure 9 in the main text were obtained from individual runs shown in Figures S2-S14, and summarized in table S1.

Table S1

eq PPh_3	mM PPh_3	k_{obs} (s^{-1})
0	0	2.18×10^{-4}
0.125	1.1	1.54×10^{-5}
0.25	2.2	1.19×10^{-5}
0.375	3.3	6.27×10^{-6}
0.5	4.4	5.28×10^{-6}
0.5	4.4	5.77×10^{-6}
0.625	5.4	4.14×10^{-6}
0.75	6.5	2.58×10^{-6}
0.75	6.5	3.14×10^{-6}
0.875	7.6	2.32×10^{-6}
1	8.7	1.88×10^{-6}
1.125	9.8	1.90×10^{-6}
1.25	10.9	1.70×10^{-6}

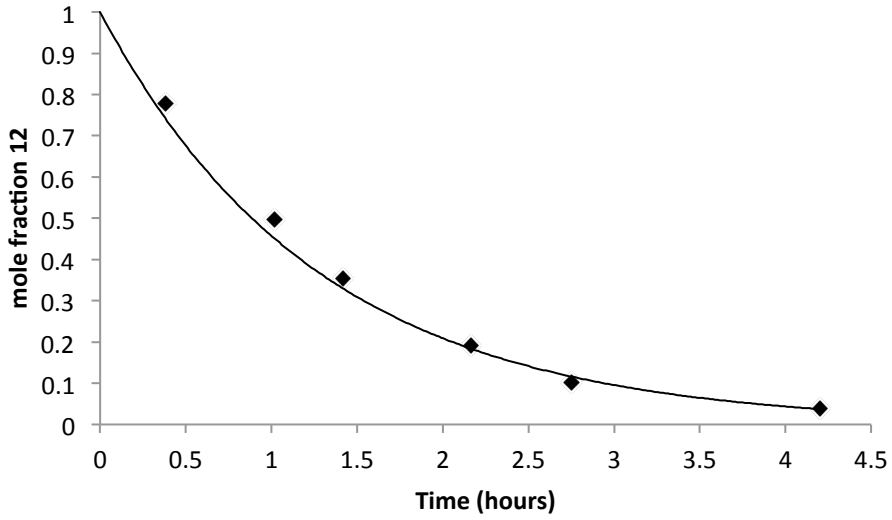


Figure S2. Conversion of **12** to **17-d_6** with no extra PPh_3 added. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 0 mM. Measured k_{obs} = 2.2 x 10^{-4} s^{-1}, with an R^2 value of 0.9937.

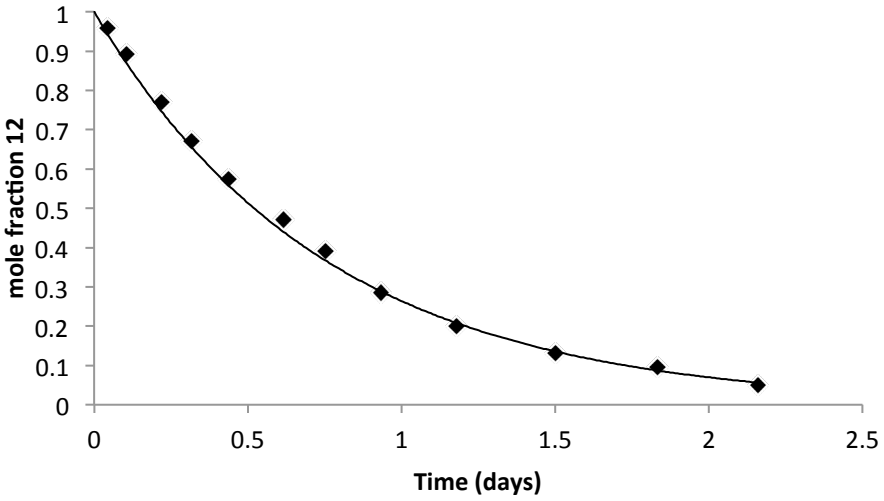


Figure S3. Conversion of **12** to **17-d_6** with 0.125 eq PPh_3 added. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 1.1 mM. Measured k_{obs} = 1.5 x 10^{-5} s^{-1}, with an R^2 value of 0.9965.

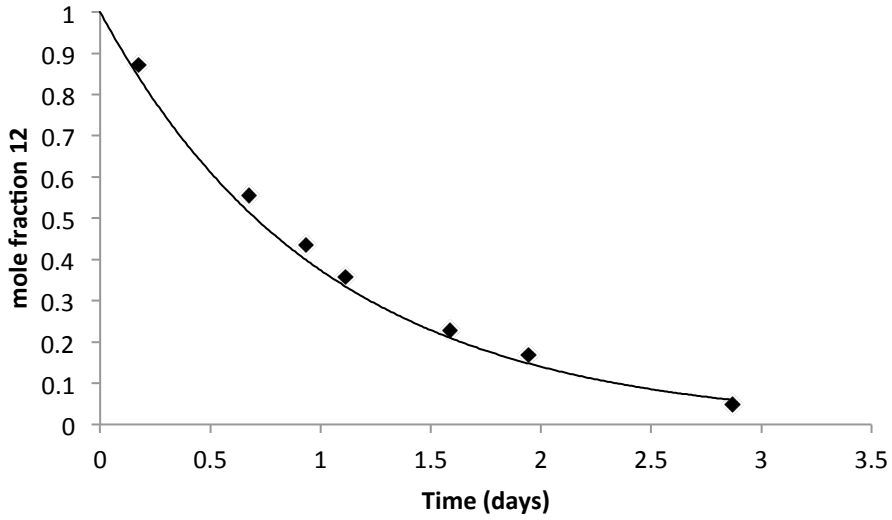


Figure S4. Conversion of **12** to **17-d_6** with 0.25 eq PPh_3 added. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 2.2 mM. Measured k_{obs} = 1.2 x 10^{-5} s^{-1}, with an R^2 value of 0.9842.

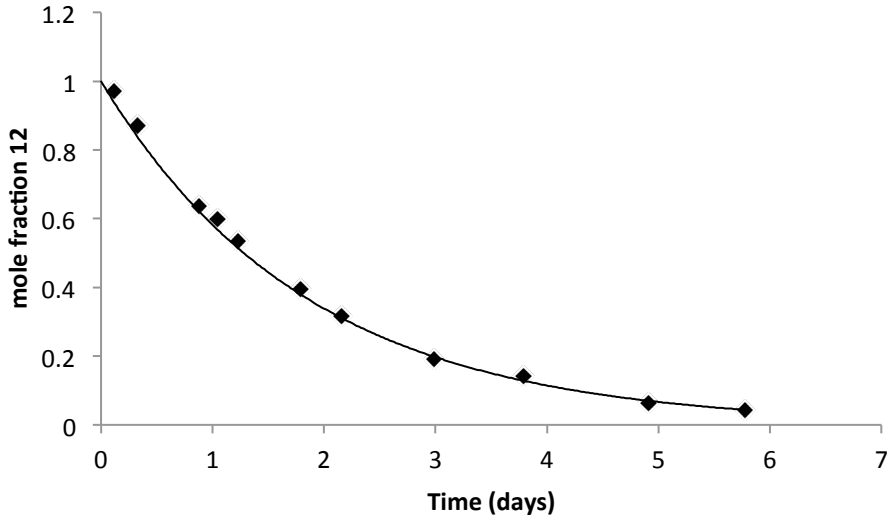


Figure S5. Conversion of **12** to **17-d_6** with 0.375 eq PPh_3 added. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 3.3 mM. Measured k_{obs} = 6.3 x 10^{-6} s^{-1}, with an R^2 value of 0.9964.

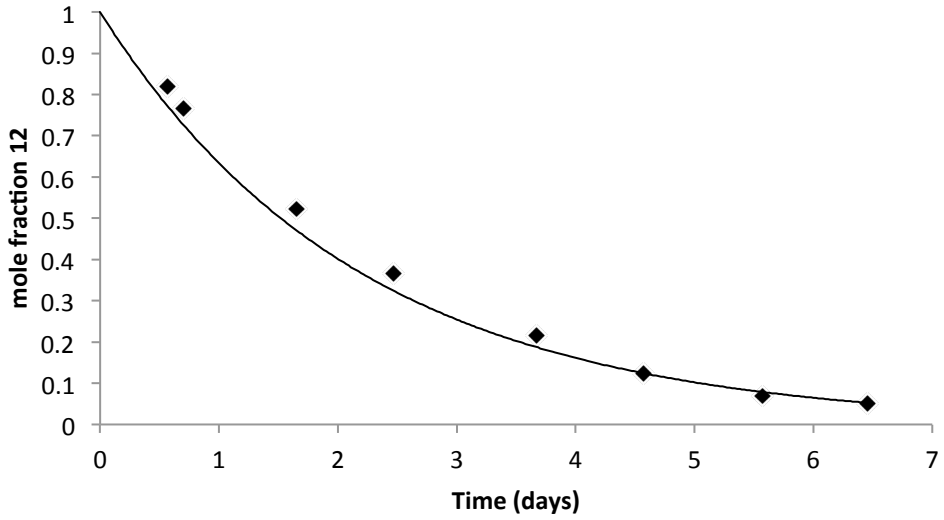


Figure S6. Conversion of **12** to **17-d_6** with 0.5 eq PPh_3 added, first run. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 4.4 mM. Measured k_{obs} = 5.3 x 10^{-6} s^{-1}, with an R^2 value of 0.9910.

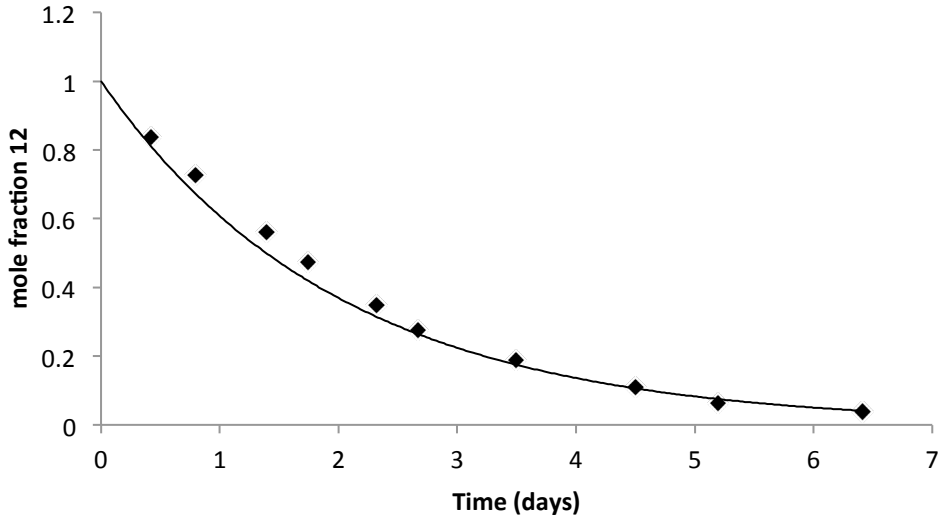


Figure S7. Conversion of **12** to **17-d_6** with 0.5 eq PPh_3 added, second run. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 4.4 mM. Measured k_{obs} = 5.8 x 10^{-6} s^{-1}, with an R^2 value of 0.9921.

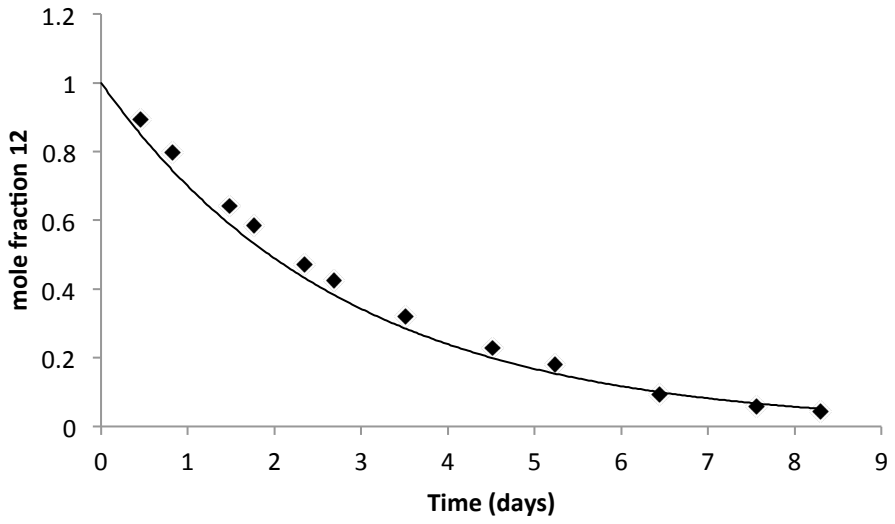


Figure S8. Conversion of **12** to **17-d_6** with 0.625 eq PPh_3 added. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 5.4 mM. Measured k_{obs} = 4.1 x 10^{-6} s^{-1}, with an R^2 value of 0.9877.

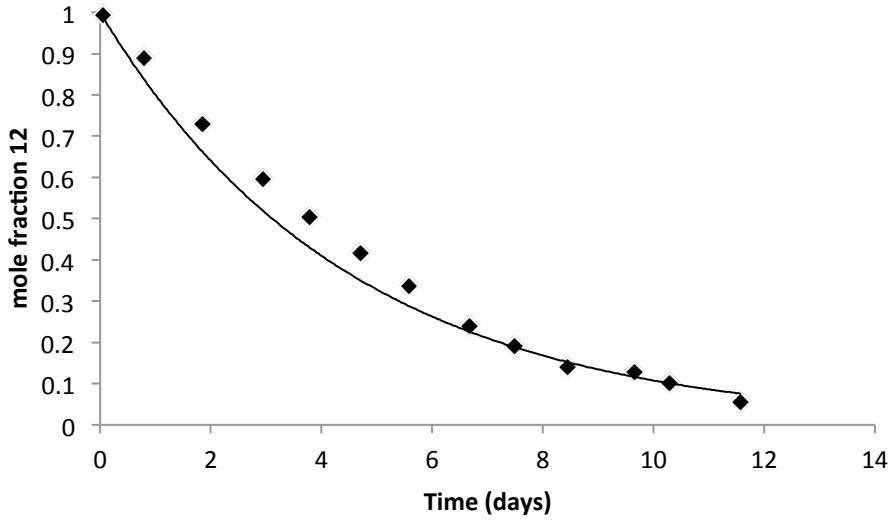


Figure S9. Conversion of **12** to **17-d_6** with 0.75 eq PPh_3 added, first run. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 6.5 mM. Measured k_{obs} = 2.6 x 10^{-6} s^{-1}, with an R^2 value of 0.9768.

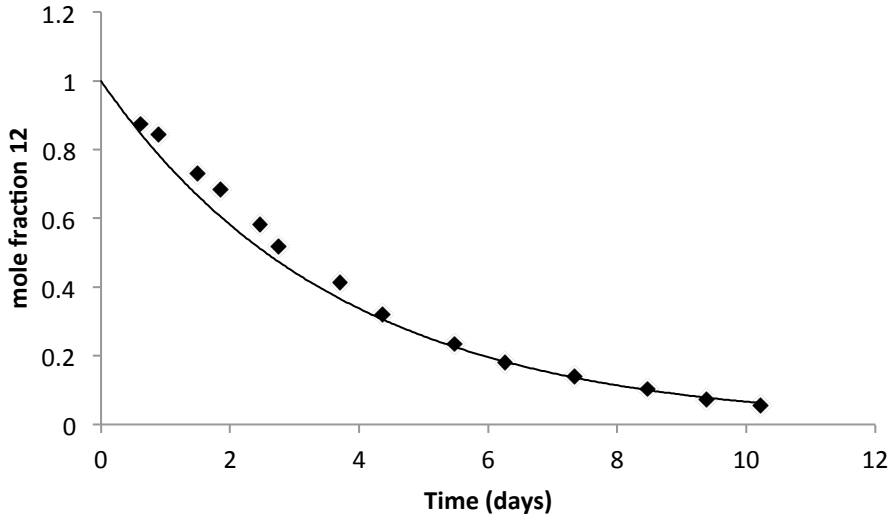


Figure S10. Conversion of **12** to **17-d_6** with 0.75 eq PPh_3 added, second run. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 6.5 mM. Measured k_{obs} = 3.1 x 10^{-6} s^{-1}, with an R^2 value of 0.9912 .

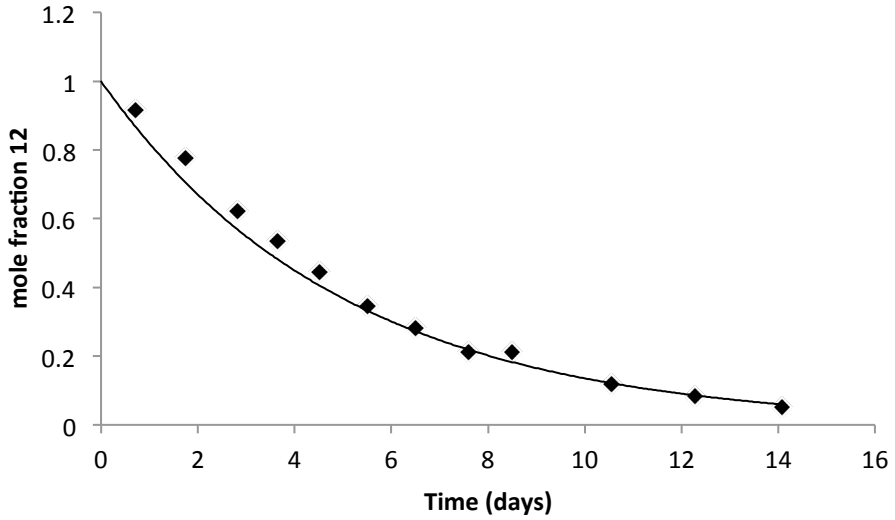


Figure S11. Conversion of **12** to **17-d_6** with 0.875 eq PPh_3 added. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 7.6 mM. Measured k_{obs} = 2.3 x 10^{-6} s^{-1}, with an R^2 value of 0.9904.

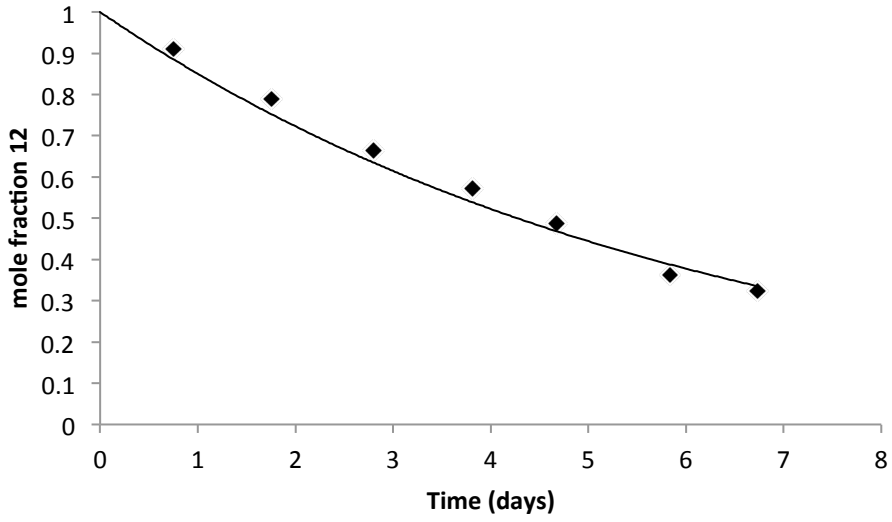


Figure S12. Conversion of **12** to **17-d_6** with 1 eq PPh_3 added. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 8.7 mM. Measured k_{obs} = 1.9 x 10^{-6} s^{-1}, with an R^2 value of 0.9821.

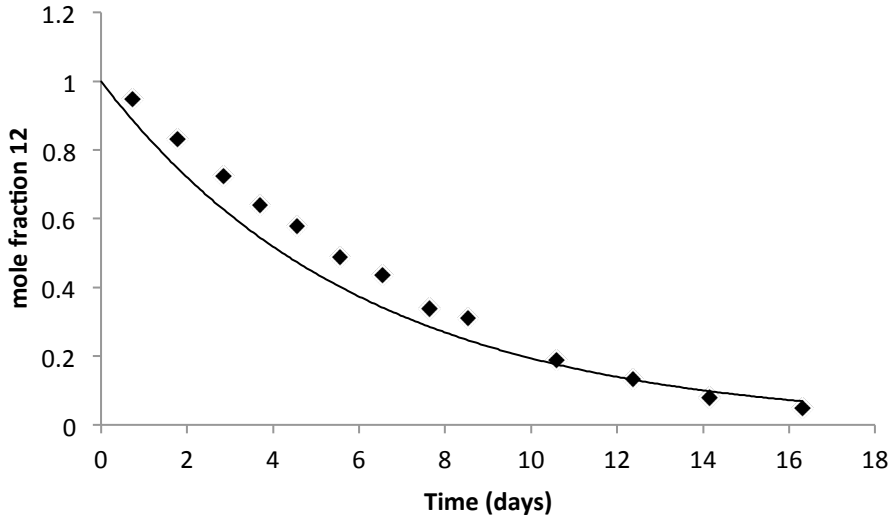


Figure S13. Conversion of **12** to **17-d_6** with 1.125 eq PPh_3 added. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 9.8 mM. Measured k_{obs} = 1.9 x 10^{-6} s^{-1}, with an R^2 value of 0.9558

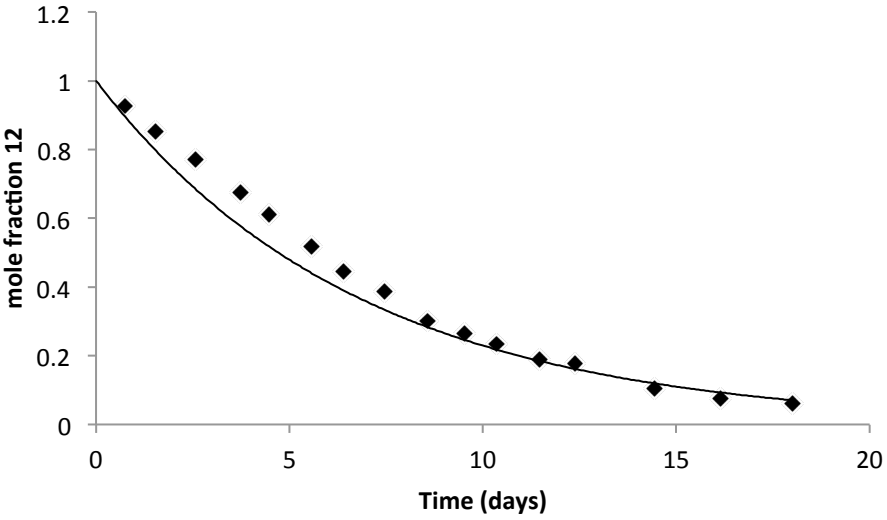
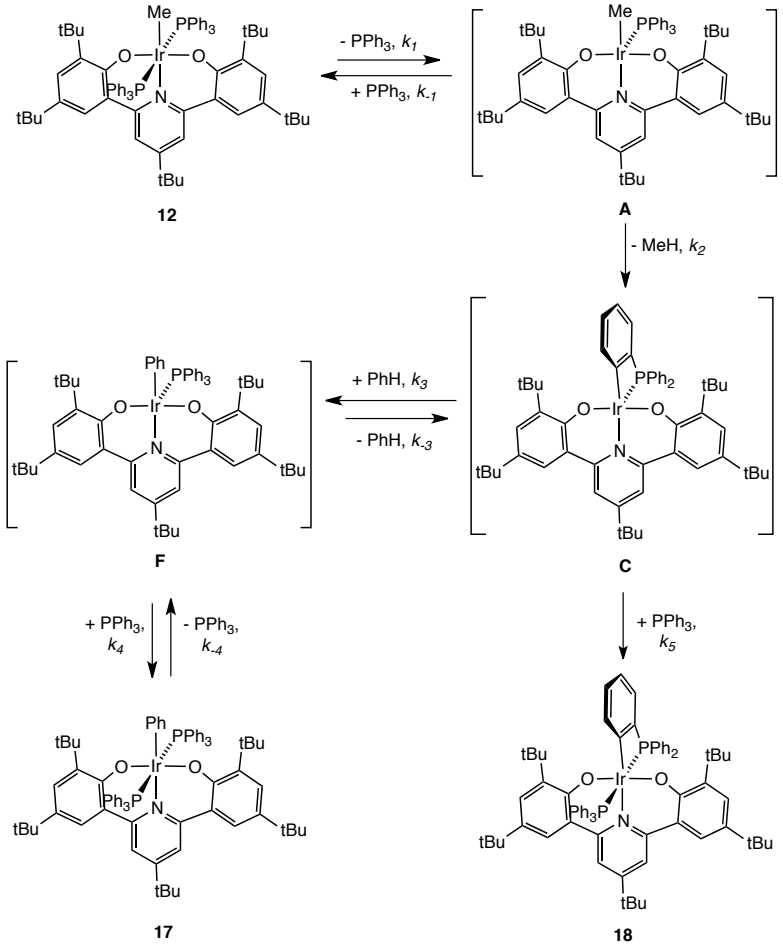


Figure S14. Conversion of **12** to **17-d_6** with 1.25 eq PPh_3 added. $[\mathbf{12}]_0$ = 8.7 mM, $[PPh_3]_0$ = 10.9 mM. Measured k_{obs} = 1.7 x 10^{-6} s^{-1}, with an R^2 value of 0.9777.

III. Derivation of Rate Laws



Scheme 9 (reproduced from main text for convenience)

Treating dissociation of L from **12** as a fast pre-equilibrium and intramolecular C-H activation of L as rate-determining, we get K_1 = [**A**][L]/[**12**] and $-d$[**12**]/dt = k_2[**A**] = (k_2K_1[**12**])/[L].

For conversion of **17** to **18**, we want to use the steady-state approximation for both **C** and **F**, which should both be present in low concentration and in rapid equilibrium with one another. This is most simply accomplished by defining a dummy variable [**X**] = [**C**] + [**F**]. For steady-state in [**X**]: 0 = d[**X**]/dt = k_{-4}[**17**] – k_4[**F**][L] – k_5[**C**][L]. Substituting [**F**] = K_3[**C**][PhH] gives k_{-4}[**17**] – k_4[**F**][L] – k_5[**C**][L] = k_{-4}[**17**] – K_3k_4[**C**][PhH][L] – k_5[**C**][L] = 0; hence [**C**] = (k_{-4}[**17**])/(k_5[L] + K_3k_4[PhH][L]). Hence the rate law for the conversion is $-d$[**17**]/dt = d[**18**]/dt = k_5[**C**][L] = ($k_{-4}k_5$[**17**])/(k_5 + K_3k_4[PhH]).

IV. Molecular Structures (of complexes not shown in main text)

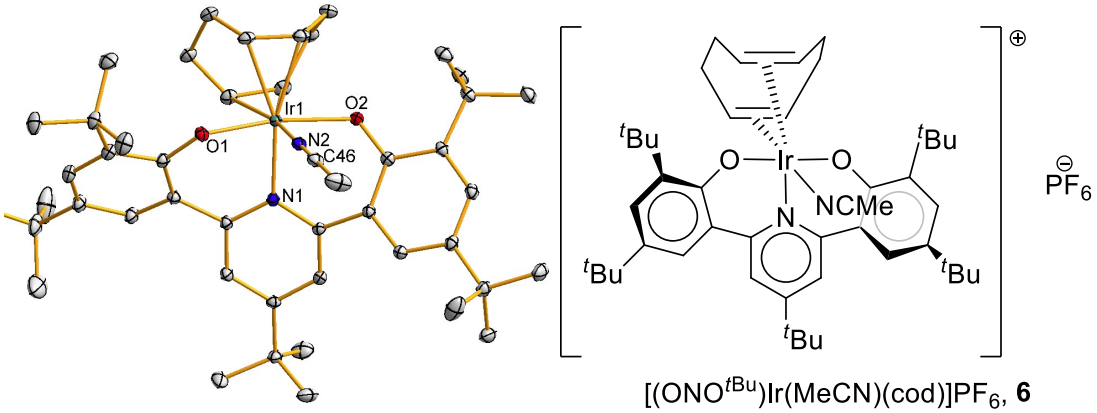


Figure S15. Crystal structure of **6**. A benzene solvent molecule and the PF_6 counterion have been removed for clarity. Selected atom distances (Å) and angles (º): Ir(1)-N(1), 2.0736(8); Ir(1)-N(2), 2.0456(8); Ir(1)-O(1), 2.0540(7); Ir(1)-O(2), 2.0849(7); N(2)-C(46), 1.1371(12); O(1)-Ir(1)-N(1), 85.86(3); O(1)-Ir(1)-N(2), 81.05(3); O(2)-Ir(1)-N(1), 89.17(3); O(2)-Ir(1)-N(2), 85.09(3); O(1)-Ir(1)-O(2), 165.29(3); N(1)-Ir(1)-N(2), 89.69(3); Ir(1)-N(2)-C(46), 173.51(8).

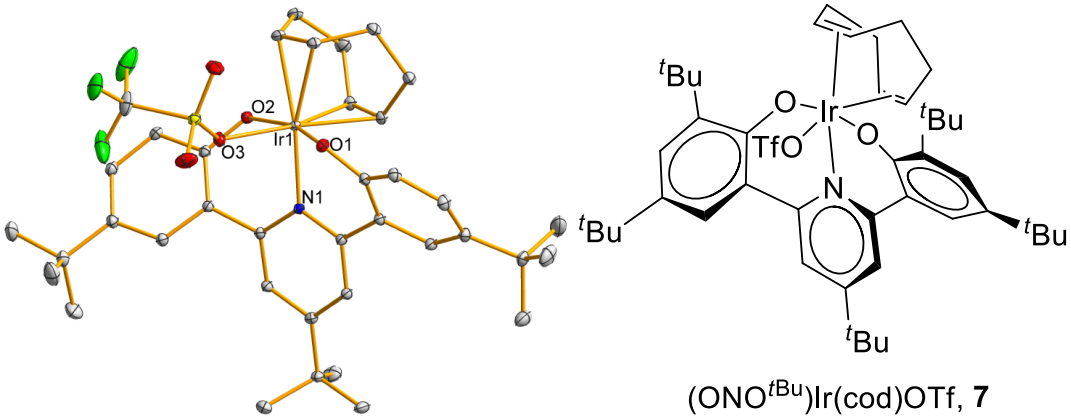


Figure S16. Crystal structure of **7**. The two tert-butyl groups ortho to the phenoxy moieties have been removed for clarity. Selected atom distances (Å) and angles (º): Ir(1)-O(1), 2.0431(6); Ir(1)-N(1), 2.0738(6); Ir(1)-O(2), 2.0836(6); Ir(1)-O(3), 2.1247(6); Ir(1)-C(39), 2.1725(8); Ir(1)-C(40), 2.1865(8); Ir(1)-C(44), 2.2592(8); Ir(1)-C(43), 2.2656(8); O(1)-Ir(1)-N(1), 84.59(2); O(1)-Ir(1)-O(2), 163.22(2); N(1)-Ir(1)-O(2), 88.90(2); O(1)-Ir(1)-O(3), 80.91(2); N(1)-Ir(1)-O(3), 87.90(2); O(2)-Ir(1)-O(3), 83.42(2); O(1)-Ir(1)-C(39), 121.97(3); N(1)-Ir(1)-C(39), 95.20(3); O(2)-Ir(1)-C(39), 73.96(3); O(3)-Ir(1)-C(39), 157.08(3); O(1)-Ir(1)-C(40), 84.60(3); N(1)-Ir(1)-C(40), 90.09(3); O(2)-Ir(1)-C(40), 110.91(3); O(3)-Ir(1)-C(40), 165.50(3); C(39)-Ir(1)-C(40), 37.42(3); O(1)-Ir(1)-C(44), 110.92(3); N(1)-Ir(1)-C(44), 164.19(3); O(2)-Ir(1)-C(44), 75.34(3); O(3)-Ir(1)-C(44), 91.51(3); C(39)-Ir(1)-C(44), 79.40(3); C(40)-Ir(1)-C(44), 94.28(3); O(1)-Ir(1)-C(43), 77.60(3); N(1)-Ir(1)-C(43), 159.93(3); O(2)-Ir(1)-C(43), 110.72(3); O(3)-Ir(1)-C(43), 98.24(3); C(39)-Ir(1)-C(43), 86.58(3); C(40)-Ir(1)-C(43), 79.18(3); C(44)-Ir(1)-C(43), 35.50(3).

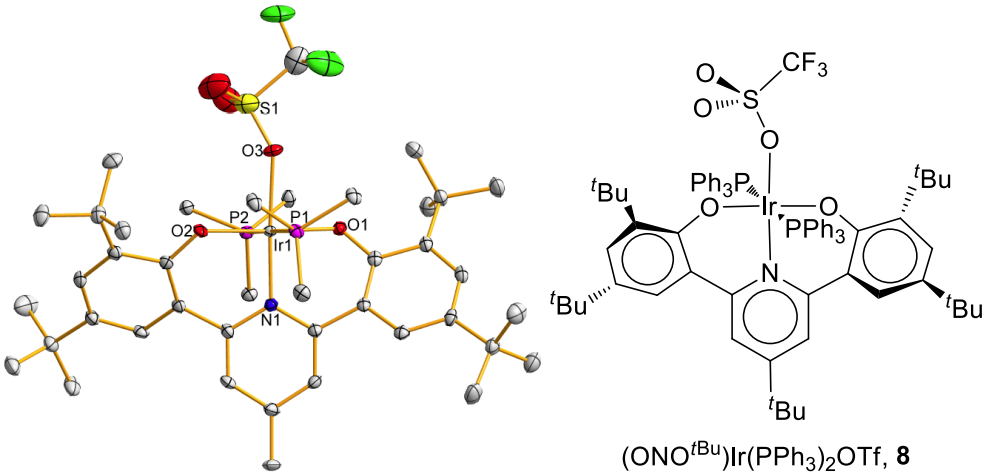


Figure S17. Crystal structure of **8**. Two benzene solvent molecules, a *tert*-butyl group's methyls, and the phosphine ligands' phenyl groups (except *ipso* carbons) have been removed for clarity. Selected atom distances (Å) and angles (º): Ir(1)-N(1), 2.001(3); Ir(1)-O(1), 2.049(2); Ir(1)-O(2), 2.051(2); Ir(1)-O(3), 2.166(2); Ir(1)-P(1), 2.4142(8); Ir(1)-P(2), 2.4165(8); N(1)-Ir(1)-O(1), 90.68(9); N(1)-Ir(1)-O(2), 91.55(9); O(1)-Ir(1)-O(2), 177.70(8); N(1)-Ir(1)-O(3), 176.28(9); O(1)-Ir(1)-O(3), 87.33(8); O(2)-Ir(1)-O(3), 90.41(8); N(1)-Ir(1)-P(1), 90.90(7); O(1)-Ir(1)-P(1), 96.69(6); O(2)-Ir(1)-P(1), 82.71(6); O(3)-Ir(1)-P(1), 86.22(6); N(1)-Ir(1)-P(2), 88.06(7); O(1)-Ir(1)-P(2), 81.27(6); O(2)-Ir(1)-P(2), 99.37(6); O(3)-Ir(1)-P(2), 94.74(6); P(1)-Ir(1)-P(2), 177.70(3).

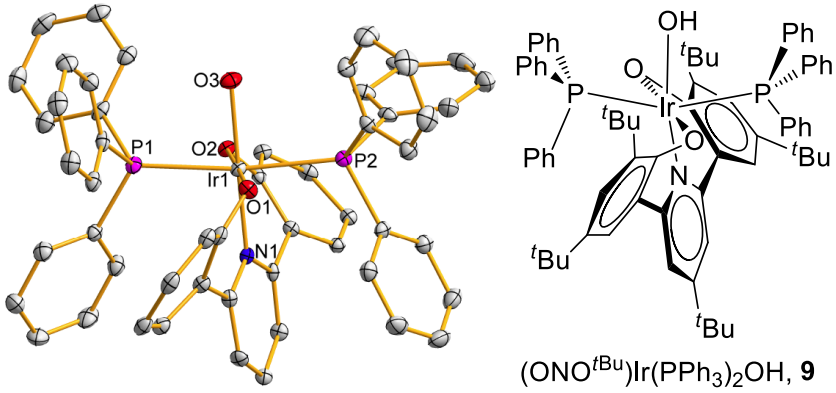


Figure S18. Crystal structure of **9**. The *tert*-butyl groups have been removed for clarity. Selected atom distances (Å) and angles (º): Ir(1)-N(1), 2.0395(14); Ir(1)-O(3), 2.0561(13); Ir(1)-O(1), 2.0624(11); Ir(1)-O(2), 2.0686(11); Ir(1)-P(1), 2.3654(5); Ir(1)-P(2), 2.3920(5); N(1)-Ir(1)-O(3), 179.30(6); N(1)-Ir(1)-O(1), 89.78(5); O(3)-Ir(1)-O(1), 90.03(5); N(1)-Ir(1)-O(2), 89.99(5); O(3)-Ir(1)-O(2), 90.22(5); O(1)-Ir(1)-O(2), 178.69(5); N(1)-Ir(1)-P(1), 97.67(4); O(3)-Ir(1)-P(1), 83.02(4); O(1)-Ir(1)-P(1), 95.33(4); O(2)-Ir(1)-P(1), 83.43(4); N(1)-Ir(1)-P(2), 90.84(4); O(3)-Ir(1)-P(2), 88.46(4); O(1)-Ir(1)-P(2), 81.46(4); O(2)-Ir(1)-P(2), 99.83(4); P(1)-Ir(1)-P(2), 170.911(15).

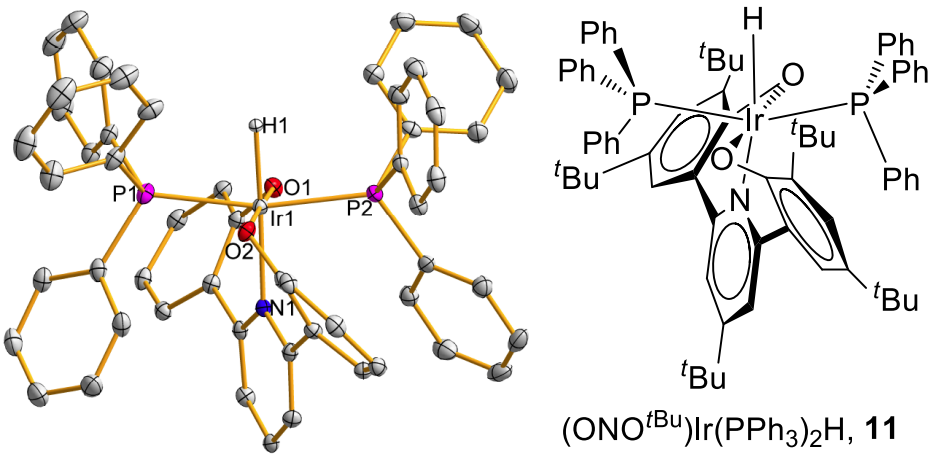


Figure S19. Crystal structure of **11**. A pentane solvent molecule and the *tert*-butyl groups have been removed for clarity. Selected atom distances (Å) and angles (º): Ir(1)-O(1), 2.0663(11); Ir(1)-O(2), 2.0764(11); Ir(1)-N(1), 2.1020(16); Ir(1)-P(2), 2.3229(5); Ir(1)-P(1), 2.3320(5); Ir(1)-H(1), 1.70(2); O(1)-Ir(1)-O(2), 176.19(5); O(1)-Ir(1)-N(1), 87.97(5); O(2)-Ir(1)-N(1), 88.25(5); O(1)-Ir(1)-P(2), 86.17(4); O(2)-Ir(1)-P(2), 94.68(3); N(1)-Ir(1)-P(2), 95.82(4); O(1)-Ir(1)-P(1), 96.13(4); O(2)-Ir(1)-P(1), 83.91(3); N(1)-Ir(1)-P(1), 97.67(4); P(2)-Ir(1)-P(1), 166.384(19); O(1)-Ir(1)-H(1), 95.6(6); O(2)-Ir(1)-H(1), 88.2(6); N(1)-Ir(1)-H(1), 176.3(7); P(2)-Ir(1)-H(1), 85.7(7); P(1)-Ir(1)-H(1),80.7(7).

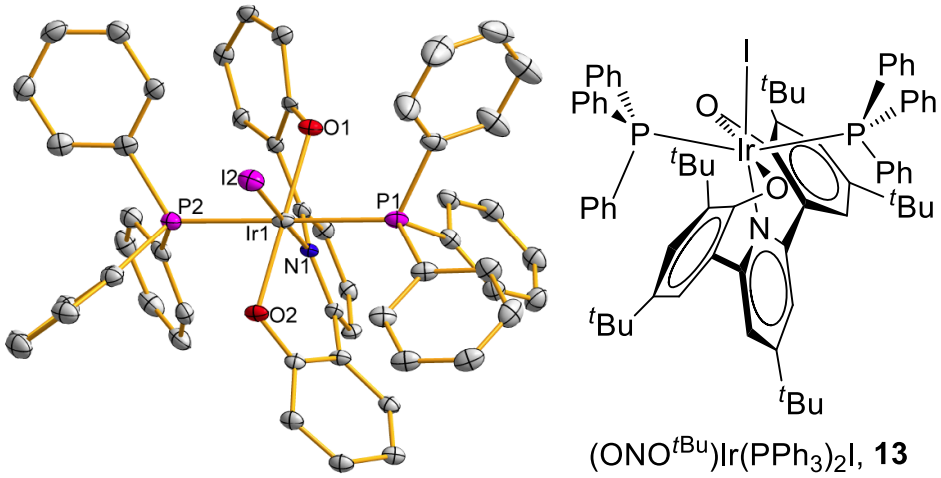


Figure S20. Crystal structure of **13**. Two pentane solvent molecules and the *tert*-butyl groups have been removed for clarity. Selected atom distances (Å) and angles (º): Ir(1)-N(1), 2.040(3); Ir(1)-O(2), 2.066(2); Ir(1)-O(1), 2.076(2); Ir(1)-P(2), 2.4233(10); Ir(1)-P(1), 2.4247(11); Ir(1)-I(2), 2.7013(3); N(1)-Ir(1)-O(2), 89.52(10); N(1)-Ir(1)-O(1), 88.88(10); O(2)-Ir(1)-O(1), 178.36(9); N(1)-Ir(1)-P(2), 89.69(9); O(2)-Ir(1)-P(2), 78.59(8); O(1)-Ir(1)-P(2), 101.03(8); N(1)-Ir(1)-P(1), 89.04(9); O(2)-Ir(1)-P(1), 102.10(8); O(1)-Ir(1)-P(1), 78.25(8); P(2)-Ir(1)-P(1), 178.55(3); N(1)-Ir(1)-I(2), 179.19(9); O(2)-Ir(1)-I(2), 90.56(6); O(1)-Ir(1)-I(2), 91.05(7); P(2)-Ir(1)-I(2), 91.12(2); P(1)-Ir(1)-I(2), 90.15(2).

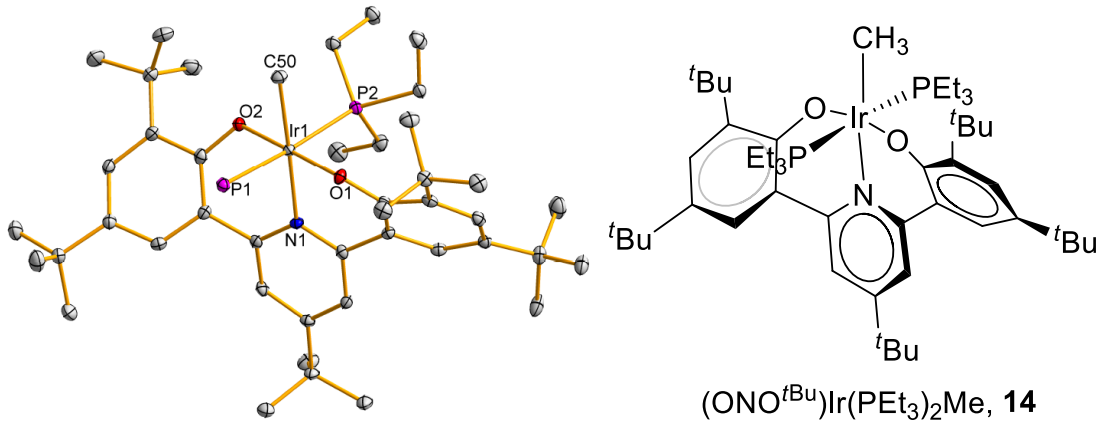


Figure S21. Crystal structure of **14**. The ethyl groups of one phosphine ligand have been removed for clarity. Selected atom distances (Å) and angles (º): Ir(1)-O(2), 2.0674(11); Ir(1)-O(1), 2.0702(11); Ir(1)-N(1), 2.1050(14); Ir(1)-C(50), 2.1154(17); Ir(1)-P(2), 2.3479(5); Ir(1)-P(1), 2.3514(5); O(2)-Ir(1)-O(1), 178.26(5); O(2)-Ir(1)-N(1), 88.65(5); O(1)-Ir(1)-N(1), 89.83(5); O(2)-Ir(1)-C(50), 91.12(6); O(1)-Ir(1)-C(50), 90.42(6); N(1)-Ir(1)-C(50), 178.40(6); O(2)-Ir(1)-P(2), 84.03(4); O(1)-Ir(1)-P(2), 95.23(4); N(1)-Ir(1)-P(2), 93.93(4); C(50)-Ir(1)-P(2), 87.61(5); O(2)-Ir(1)-P(1), 97.78(4); O(1)-Ir(1)-P(1), 83.10(4); N(1)-Ir(1)-P(1), 91.40(4); C(50)-Ir(1)-P(1), 87.07(5); P(2)-Ir(1)-P(1), 174.416(16).

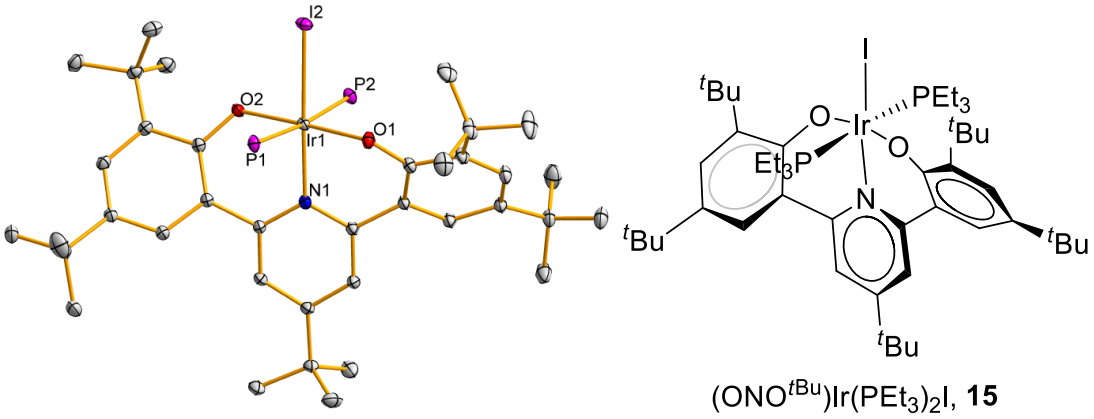
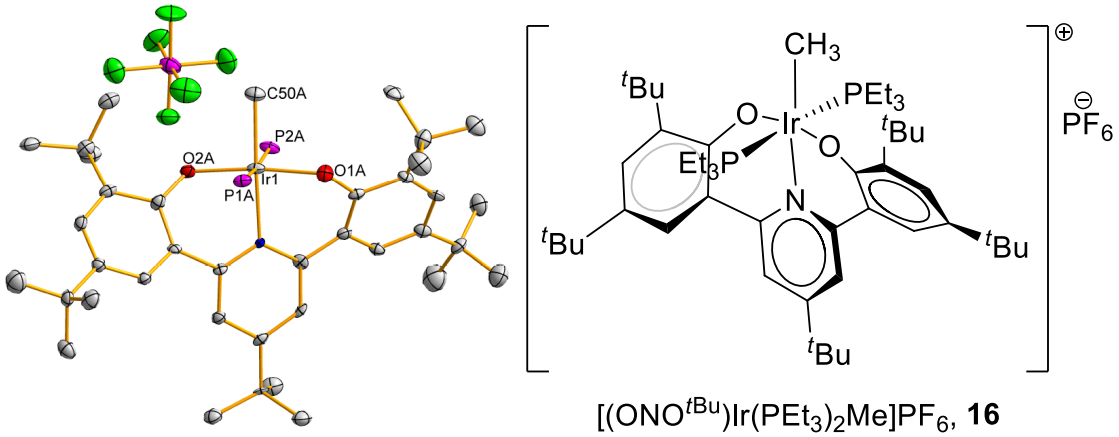
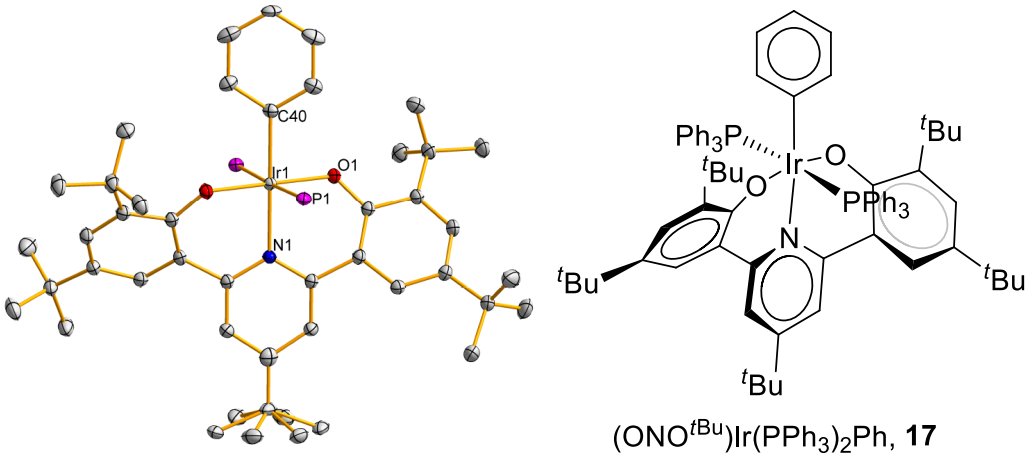


Figure S22. Crystal structure of **15**. The ethyl groups of the phosphine ligands have been removed for clarity. Selected atom distances (Å) and angles (º): Ir(1)-N(1), 2.0619(13); Ir(1)-O(2), 2.0648(11); Ir(1)-O(1), 2.0661(11); Ir(1)-C(50), 2.148(7); Ir(1)-P(1), 2.3711(4); Ir(1)-P(2), 2.3722(4); Ir(1)-I(2), 2.6625(3); N(1)-Ir(1)-O(2), 89.86(5); N(1)-Ir(1)-O(1), 88.67(5); O(2)-Ir(1)-O(1), 178.36(5); N(1)-Ir(1)-C(50), 177.12(15); O(2)-Ir(1)-C(50), 89.65(17); O(1)-Ir(1)-C(50), 91.86(17); N(1)-Ir(1)-P(1), 93.81(4); O(2)-Ir(1)-P(1), 95.64(3); O(1)-Ir(1)-P(1), 83.74(3); C(50)-Ir(1)-P(1), 89.06(15); N(1)-Ir(1)-P(2), 91.30(4); O(2)-Ir(1)-P(2), 82.36(3); O(1)-Ir(1)-P(2), 98.40(3); C(50)-Ir(1)-P(2), 85.82(15); P(1)-Ir(1)-P(2), 174.510(14); N(1)-Ir(1)-I(2), 178.40(4); O(2)-Ir(1)-I(2), 91.65(3); O(1)-Ir(1)-I(2), 89.83(3); C(50)-Ir(1)-I(2), 3.05(16); P(1)-Ir(1)-I(2), 86.571(11); P(2)-Ir(1)-I(2), 88.374(11).



[(ONO$^{t\text{Bu}}$)Ir(PEt$_3$)$_2$Me]PF$_6$, **16**

Figure S23. Crystal structure of one of the molecules of **16** in the unit cell. The unit cell has 4 iridium-containing molecules total; this figure only shows one of them (the A molecule, see tables **S54-S57**). In addition, ethyl groups on the phosphine ligands, as well as the six benzene molecules per unit cell, have been removed for clarity. Selected atom distances (Å) and angles (º): Ir(1)-O(2A), 1.994(5); Ir(1)-O(1A), 2.011(5); Ir(1)-C(50A), 2.101(8); Ir(1)-N(1A), 2.129(7); Ir(1)-P(2A), 2.400(2); Ir(1)-P(1A), 2.418(2); O(2A); Ir(1)-O(1A), 173.5(2); O(2A)-Ir(1)-C(50A), 94.2(3); O(1A)-Ir(1)-C(50A), 92.3(3); O(2A)-Ir(1)-N(1A), 87.4(2); O(1A)-Ir(1)-N(1A), 86.1(2); C(50A)-Ir(1)-N(1A), 177.4(3); O(2A)-Ir(1)-P(2A), 82.62(17); O(1A)-Ir(1)-P(2A), 98.06(18); C(50A)-Ir(1)-P(2A), 84.4(2); N(1A)-Ir(1)-P(2A), 93.78(18); O(2A)-Ir(1)-P(1A), 98.16(17); O(1A)-Ir(1)-P(1A), 81.81(18); C(50A)-Ir(1)-P(1A), 89.8(2); N(1A)-Ir(1)-P(1A), 91.96(18); P(2A)-Ir(1)-P(1A), 174.24(8).



(ONO$^{t\text{Bu}}$)Ir(PPh$_3$)$_2$Ph, **17**

Figure S24. Crystal structure of (ONO$^{t\text{Bu}}$)Ir(PPh$_3$)$_2$Ph, **17**. A benzene and a pentane solvent molecule, as well as the phosphine phenyl groups, have been removed for clarity. The molecule is symmetric about the iridium center. Selected atom distances (Å) and angles (º): Ir(1)-O(1), 2.0744(12); Ir(1)-C(40), 2.074(3); Ir(1)-N(1), 2.103(2); Ir(1)-P(1), 2.3921(6); O(1)-Ir(1)-C(40), 90.05(4); O(1)-Ir(1)-O(1)#1, 179.91(8); C(40)-Ir(1)-O(1)#1, 90.04(4); O(1)-Ir(1)-N(1), 89.95(4); C(40)-Ir(1)-N(1), 180.0; O(1)#1-Ir(1)-N(1), 89.96(4); O(1)-Ir(1)-P(1)#1, 97.70(4); C(40)-Ir(1)-P(1)#1, 88.831(13); O(1)#1-Ir(1)-P(1)#1, 82.30(4); N(1)-Ir(1)-P(1)#1, 91.169(13); O(1)-Ir(1)-P(1), 82.30(4); C(40)-Ir(1)-P(1), 88.829(13); O(1)#1-Ir(1)-P(1), 97.70(4); N(1)-Ir(1)-P(1), 91.171(13); P(1)#1-Ir(1)-P(1); 177.66(3).

V. Crystallographic Data for All Complexes

	3	4	5	6
Empirical formula	$C_{51}H_{75}NO_7NaIr$	$C_{90}H_{126}N_2O_4Na_2Ir_2 \bullet C_4H_{10}O$	$C_{53}H_{75}NO_2Ir_2$	$[C_{47}H_{66}N_2O_2Ir]^+ [PF_6]^- \bullet C_6H_6$
Formula weight	1029.31	1804.43	1142.54	1106.30
Crystal System	Monoclinic	Monoclinic	Monoclinic	Triclinic
Lattice Parameters				
***a* (Å)**	25.4702(16)	29.8716(11)	9.5497(4)	11.0592(5)
***b* (Å)**	11.7637(9)	14.4205(5)	22.3182(9)	11.8291(5)
***c* (Å)**	23.8372(15)	24.4163(15)	22.9384(10)	20.4215(9)
α (deg)	90	90	90	105.154(2)
β (deg)	120.162(2)	123.7310(10)	92.086(2)	97.156(2)
γ (deg)	90	90	90	95.370(2)
V (Å^3)	6175.20(73)	8747.0(7)	4885.7(4)	2536.27(19)
Space Group	C2	C2/*c*	$P2_1/n$	P-1
Z value	4	4	4	2
ρ_{calc} (g/cm^3)	1.107	1.370	1.553	1.449
μ (mm^{-1})	2.21	3.100	5.481	2.727
Temperature (K)	100(2)	100(2)	100(2)	100(2)
θ range (deg)	max. 2θ = 61.14	1.66 to 35.19	1.82 to 35.82	1.80 to 40.84
No. Obs. (I > 2σ(I))	7932	15255	19264	26070
No. parameters	246	485	533	874
Goodness of fit	5.251	3.747	1.885	1.957
Max. shift in cycle	0.460	0.003	0.007	0.016
Residuals*: R1; wR2	0.1446; 0.3116	0.0314; 0.0719	0.0355; 0.0535	0.0206; 0.0392
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
max/min		0.7469; 0.5672	0.7470; 0.5076	0.7480; 0.5945
Largest peak & hole (e$^-$/ Å^3)	20.27; -11.46	2.370; -1.617	2.894; -2.135	2.557; -1.524

*$R = \Sigma_{hkl}(||F_{obs}| - |F_{calc}||)/\Sigma_{hkl}|F_{obs}|$; $R_w = [\Sigma_{hkl}w(|F_{obs}| - |F_{calc}|)^2/\Sigma_{hkl}wF_{obs}^2]^{1/2}$, $w = 1/\sigma^2(F_{obs})$; GOF = $[\Sigma_{hkl}w(|F_{obs}| - |F_{calc}|)^2/(n_{data} - n_{vari})]^{1/2}$.

	7	8	9	10
Empirical formula	$C_{46}H_{63}F_3NO_5SIr$ • 1.5(C_6H_6)	$C_{74}H_{81}F_3NO_5P_2SIr$ • 0.53(C_5H_{12}) • 1.47(C_6H_6)	$C_{73}H_{82}NO_3P_2Ir$	$C_{73}H_{81}NO_2P_2ClIr$ • 5(CH_2Cl_2)
Formula weight	1108.40	1560.64	1275.54	1718.61
Crystal System	Triclinic	Monoclinic	Monoclinic	Monoclinic
Lattice Parameters				
***a* (Å)**	11.7099(4)	12.9942(5)	13.0223(4)	19.3956(9)
***b* (Å)**	13.1880(5)	22.9825(9)	21.0636(7)	13.1877(6)
***c* (Å)**	17.2153(6)	25.8969(9)	22.7792(8)	31.5557(15)
α (deg)	86.059(2)	90	90	90
β (deg)	72.263(2)	103.513(2)	99.1960(10)	106.611(2)
γ (deg)	87.034(2)	90	90	90
V (Å^3)	2524.87(16)	7519.7(5)	6167.9(4)	7734.6(6)
Space Group	P-1	$P2_1/n$	$P2_1/n$	$P2_1/c$
Z value	2	4	4	4
ρ_{calc} (g/cm^3)	1.458	1.379	1.374	1.476
μ (mm^{-1})	2.744	1.906	2.265	2.194
Temperature (K)	100(2)	100(2)	100(2)	100(2)
θ range (deg)	1.55 to 43.59	1.84 to 31.76	2.41 to 29.67	1.35 to 37.99
No. Obs. (I > 2σ(I))	34153	18398	14018	32658
No. parameters	883	966	1049	871
Goodness of fit	1.536	2.750	1.713	2.152
Max. shift in cycle	0.015	0.002	0.004	0.011
Residuals*: R1; wR2	0.0221; 0.0381	0.0463; 0.0958	0.0238; 0.0373	0.0340; 0.0589
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
max/min	0.7486; 0.6139	0.7463; 0.6010	0.7459; 0.6381	0.7474; 0.6430
Largest peak & hole (e$^-$/ Å^3)	2.541; -1.556	3.915; -2.838	2.894; -0.696	3.136; -2.303

	11	**12**	**13**	**14**
Empirical formula	$C_{73}H_{82}NO_2P_2Ir \bullet C_5H_{12}$	$C_{74}H_{84}NO_2P_2Ir$	$C_{73}H_{81}INO_2P_2Ir \bullet 2(C_5H_{12})$	$C_{50}H_{84}NO_2P_2Ir$
Formula weight	1331.68	1273.56	1529.72	985.32
Crystal System	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Lattice Parameters				
***a* (Å)**	16.8289(8)	13.1981(7)	14.4250(5)	12.2897(7)
***b* (Å)**	23.8694(10)	20.9991(9)	19.4180(6)	35.3664(19)
***c* (Å)**	17.4749(8)	22.8801(12)	26.3735(9)	11.4244(6)
α (deg)	90	90	90	90
β (deg)	102.373(2)	100.388(3)	99.362(2)	93.830(2)
γ (deg)	90	90	90	90
V (Å^3)	6856.5(5)	6237.2(5)	7288.9(4)	4954.4(5)
Space Group	$P2_1/n$	$P2_1/n$	$P2_1/c$	$P2_1/c$
Z value	4	4	4	4
ρ_{calc} (g/cm^3)	1.290	1.356	1.394	1.321
μ (mm^{-1})	2.040	2.239	2.346	2.796
Temperature (K)	100(2)	100(2)	100(2)	100(2)
θ range (deg)	1.47 to 33.55	1.66 to 29.33	1.57 to 28.67	1.76 to 27.89
No. Obs. (I > 2σ(I))	19762	10617	15318	10841
No. parameters	1086	737	848	527
Goodness of fit	2.140	1.268	2.742	1.824
Max. shift in cycle	0.004	0.003	0.002	0.003
Residuals*: R1; wR2	0.0310; 0.0519	0.0387; 0.0478	0.0482; 0.0750	0.0188; 0.0366
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
max/min	0.7466; 0.6219	0.7459; 0.6362	0.4314; 0.3230	0.7456; 0.6727
Largest peak & hole (e$^-$/ Å^3)	2.907; -2.314	1.724; -1.487	1.880; -2.150	0.633; -0.778

	15	**16**	**17**	**18**
Empirical formula	$0.67(C_{49}H_{80}INO_2P_2Ir)$ $0.33(C_{50}H_{83}NO_2P_2Ir)$	$C_{50}H_{84}NO_2F_6P_3Ir$	$C_{79}H_{86}NO_2P_2Ir \bullet 2(C_6H_6)$	$C_{73}H_{80}NO_2P_2Ir$
Formula weight	1097.19	1130.29	745.92	1257.52
Crystal System	Monoclinic	Triclinic	Orthorhombic	Monoclinic
Lattice Parameters				
***a* (Å)**	12.2460(6)	21.3347(12)	16.0771(8)	41.3489(19)
***b* (Å)**	35.7358(18)	21.4843(12)	20.5290(10	18.8871(9)
***c* (Å)**	11.4544(6)	26.6258(14)	23.1672(11)	20.6067(9)
α (deg)	90	81.834(3)	90	90
β (deg)	93.490(2)	85.853(3)	90	111.731(2)
γ (deg)	90	89.425(3)	90	90
V ($Å^3$)	6856.5(5)	12048.9(12)	7646.3(6)	14949.3(12)
Space Group	$P2_1/c$	P-1	P*bcn*	C2/*c*
Z value	4	8	8	8
ρ_{calc} (g/cm^3)	1.457	1.246	1.296	1.117
μ (mm^{-1})	3.386	2.35	1.837	1.867
Temperature (K)	100(2)	100(2)	100(2)	100(2)
θ range (deg)	1.87 to 40.01	max. 2θ = 55.96	1.76 to 37.38	1.47 to 32.01
No. Obs. (I > 2σ(I))	25951	29044	13314	20406
No. parameters	537	2305	417	758
Goodness of fit	1.448	10.016	3.326	2.133
Max. shift in cycle	0.010	0.300	0.001	0.008
Residuals*: R1; wR2	0.0344; 0.0620	0.5300; 0.8415	0.0443; 0.0804	0.0311; 0.0569
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
max/min	0.7479; 0.6295		0.7473; 0.6479	0.7463; 0.6478
Largest peak & hole (e^-/ $Å^3$)	2.448; -2.844	85.87; -15.20	4.097; -2.794	1.457; -0.873

	19	**$(ONO^{tBu})Ir(PEt_3)_2Cl$**
Empirical formula	$C_{114}H_{136}Li_2N_4O_4P_2Ir_2$	$C_{49}H_{81}ClNO_2P_2Ir$
Formula weight	2086.49	1005.74
Crystal System	Triclinic	Monoclinic
Lattice Parameters		
***a* (Å)**	16.4557(8)	12.2623(6)
***b* (Å)**	17.2824(8)	35.4340(17)
***c* (Å)**	21.7560(10)	11.3773(6)
α (deg)	93.951(2)	90
β (deg)	96.184(3)	93.368(2)
γ (deg)	101.190(3)	90
V ($Å^3$)	6008.7(5)	4934.9(4)
Space Group	P-1	$P2_1/c$
Z value	2	4
ρ_{calc} (g/cm^3)	1.153	1.354
μ (mm^{-1})	2.284	2.861
Temperature (K)	100(2)	100(2)
θ range (deg)	2.34 to 34.09	1.88 to 39.87
No. Obs. (I > 2σ(I))	30107	26158
No. parameters	1176	526
Goodness of fit	2.866	2.079
Max. shift in cycle	0.007	0.003
Residuals*: R1; wR2	0.0335; 0.0589	0.0371; 0.0602
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
max/min	0.7461; 0.6684	0.7478; 0.5515
Largest peak & hole (e^-/ $Å^3$)	1.933; -1.882	2.623; -2.981

VI. Crystallographic Details for All Complexes

Pyridine-activated complex 3

Because of the sensitivity of the crystal to the atmosphere, the x-ray structure was only of sufficient quality to establish connectivity.

[NaIr(cod)(ONO^{tBu})]$_2$, 4

Crystals were mounted on a glass fiber using Paratone oil, then placed on the diffractometer under a nitrogen stream at 100K.

The crystal contains petroleum ether as a solvent of crystallization. The model contains one molecule of disordered solvent with oxygen on the two-fold axis. The Iridium complex itself sits on a center of symmetry and therefore the atoms list contains half of the atoms.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **4**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ir(1)	3575(1)	5665(1)	9646(1)	14(1)	1
Na(1)	4914(1)	5042(1)	10521(1)	25(1)	1
O(1)	4104(1)	4609(1)	10251(1)	16(1)	1
O(2)	4763(1)	6120(1)	9804(1)	18(1)	1
N(1)	3733(1)	5070(1)	8972(1)	12(1)	1
C(1)	3858(1)	3786(2)	10019(1)	14(1)	1
C(2)	3889(1)	3088(2)	10452(1)	14(1)	1

C(3)	3566(1)	2312(2)	10167(1)	14(1)	1
C(4)	3231(1)	2154(2)	9488(1)	13(1)	1
C(5)	3255(1)	2798(2)	9089(1)	12(1)	1
C(6)	3568(1)	3590(2)	9336(1)	12(1)	1
C(7)	3654(1)	4144(2)	8891(1)	13(1)	1
C(8)	3675(1)	3682(2)	8402(1)	14(1)	1
C(9)	3780(1)	4156(2)	7986(1)	13(1)	1
C(10)	3889(1)	5101(2)	8111(1)	13(1)	1
C(11)	3874(1)	5543(2)	8604(1)	12(1)	1
C(12)	4006(1)	6530(2)	8757(1)	11(1)	1
C(13)	3712(1)	7189(2)	8273(1)	13(1)	1
C(14)	3799(1)	8134(2)	8408(1)	14(1)	1
C(15)	4182(1)	8368(2)	9065(1)	15(1)	1
C(16)	4494(1)	7732(2)	9566(1)	14(1)	1
C(17)	4438(1)	6772(2)	9406(1)	13(1)	1
C(18)	4280(1)	3159(2)	11206(1)	16(1)	1
C(19)	4163(1)	4006(2)	11479(1)	35(1)	1
C(20)	4242(1)	2316(2)	11550(1)	32(1)	1
C(21)	4855(1)	3212(2)	11377(1)	32(1)	1
C(22)	2876(1)	1291(2)	9223(1)	18(1)	1
C(23)	2444(1)	1359(2)	9389(2)	30(1)	1
C(24)	3208(1)	414(2)	9533(2)	29(1)	1
C(25)	2584(1)	1203(2)	8471(1)	26(1)	1
C(26)	3780(1)	3673(2)	7426(1)	17(1)	1
C(27)	3666(1)	2641(2)	7390(1)	23(1)	1
C(28)	4335(1)	3820(2)	7527(1)	22(1)	1
C(29)	3340(1)	4111(2)	6775(1)	24(1)	1
C(30)	3457(1)	8851(2)	7873(1)	21(1)	1
C(31)	2877(1)	8817(2)	7695(2)	33(1)	1

C(32)	3671(1)	9841(2)	8090(1)	30(1)	1
C(33)	3463(1)	8628(2)	7258(1)	36(1)	1
C(34)	4904(1)	8083(2)	10269(1)	17(1)	1
C(35)	5455(1)	8197(2)	10363(1)	27(1)	1
C(36)	4734(1)	9023(2)	10394(1)	26(1)	1
C(37)	4965(1)	7410(2)	10797(1)	28(1)	1
C(38)	3586(1)	6254(2)	10434(1)	22(1)	1
C(39)	3169(1)	5592(2)	10118(1)	20(1)	1
C(40)	2581(1)	5857(2)	9689(2)	30(1)	1
C(41)	2391(1)	5911(2)	8962(1)	30(1)	1
C(42)	2832(1)	6204(2)	8882(1)	22(1)	1
C(43)	3186(1)	6949(2)	9207(1)	23(1)	1
C(44)	3145(1)	7599(2)	9665(2)	28(1)	1
C(45)	3488(1)	7287(2)	10381(2)	30(1)	1
O(50)	5000	9592(9)	2500	343(8)	1
C(51A)	4416(1)	9618(9)	2089(5)	21(3)	0.208(9)
C(52A)	4227(6)	9890(50)	1377(9)	320(40)	0.208(9)
C(51B)	4592(2)	8974(5)	2005(4)	115(3)	0.792(9)
C(52B)	4082(1)	9544(6)	1511(3)	103(3)	0.792(9)

Table S3. Selected bond lengths [Å] and angles [°] for **4.**

Ir(1)-C(38)	2.088(3)	C(38)-Ir(1)-C(39)	39.46(10)
Ir(1)-C(39)	2.090(2)	C(38)-Ir(1)-O(1)	91.52(9)
Ir(1)-O(1)	2.0990(16)	C(39)-Ir(1)-O(1)	90.96(8)
Ir(1)-C(42)	2.099(2)	C(38)-Ir(1)-C(42)	97.80(11)
Ir(1)-N(1)	2.1274(19)	C(39)-Ir(1)-C(42)	81.82(10)
Ir(1)-C(43)	2.132(2)	O(1)-Ir(1)-C(42)	154.83(9)
Ir(1)-Na(1)	3.4465(10)	C(38)-Ir(1)-N(1)	168.64(9)
		C(39)-Ir(1)-N(1)	148.52(9)
		O(1)-Ir(1)-N(1)	81.27(7)
		C(42)-Ir(1)-N(1)	92.35(9)
		C(38)-Ir(1)-C(43)	80.45(10)
		C(39)-Ir(1)-C(43)	89.89(10)
		O(1)-Ir(1)-C(43)	166.20(9)
		C(42)-Ir(1)-C(43)	38.70(10)
		N(1)-Ir(1)-C(43)	104.78(9)
		C(38)-Ir(1)-Na(1)	96.67(8)
		C(39)-Ir(1)-Na(1)	118.33(7)
		O(1)-Ir(1)-Na(1)	38.13(5)
		C(42)-Ir(1)-Na(1)	159.57(8)
		N(1)-Ir(1)-Na(1)	72.25(5)
		C(43)-Ir(1)-Na(1)	131.26(8)

Table S4. Bond lengths [Å] and angles [°] for **4**.

Ir(1)-C(38)	2.088(3)	C(9)-C(10)	1.395(3)
Ir(1)-C(39)	2.090(2)	C(9)-C(26)	1.536(3)
Ir(1)-O(1)	2.0990(16)	C(10)-C(11)	1.387(3)
Ir(1)-C(42)	2.099(2)	C(11)-C(12)	1.468(3)
Ir(1)-N(1)	2.1274(19)	C(11)-Na(1)#1	3.130(2)
Ir(1)-C(43)	2.132(2)	C(12)-C(13)	1.386(3)
Ir(1)-Na(1)	3.4465(10)	C(12)-C(17)	1.423(3)
Na(1)-O(2)	2.193(2)	C(13)-C(14)	1.393(3)
Na(1)-O(1)	2.2145(19)	C(14)-C(15)	1.399(3)
Na(1)-O(2)#1	2.284(2)	C(14)-C(30)	1.529(3)
Na(1)-Na(1)#1	2.864(2)	C(15)-C(16)	1.392(3)
O(1)-C(1)	1.344(3)	C(16)-C(17)	1.424(3)
O(2)-C(17)	1.312(3)	C(16)-C(34)	1.539(3)
O(2)-Na(1)#1	2.284(2)	C(18)-C(20)	1.517(4)
N(1)-C(7)	1.352(3)	C(18)-C(19)	1.523(4)
N(1)-C(11)	1.366(3)	C(18)-C(21)	1.526(3)
C(1)-C(6)	1.416(3)	C(22)-C(24)	1.523(4)
C(1)-C(2)	1.426(3)	C(22)-C(25)	1.539(3)
C(2)-C(3)	1.386(3)	C(22)-C(23)	1.555(4)
C(2)-C(18)	1.541(3)	C(26)-C(27)	1.519(4)
C(3)-C(4)	1.400(3)	C(26)-C(29)	1.527(3)
C(4)-C(5)	1.376(3)	C(26)-C(28)	1.550(3)
C(4)-C(22)	1.527(3)	C(30)-C(32)	1.532(4)
C(5)-C(6)	1.384(3)	C(30)-C(31)	1.536(4)
C(6)-C(7)	1.482(3)	C(30)-C(33)	1.546(4)
C(7)-C(8)	1.399(3)	C(34)-C(36)	1.537(4)
C(8)-C(9)	1.395(3)	C(34)-C(35)	1.539(3)

C(34)-C(37)	1.542(4)	C(42)-Ir(1)-C(43)	38.70(10)
C(38)-C(39)	1.410(4)	N(1)-Ir(1)-C(43)	104.78(9)
C(38)-C(45)	1.510(4)	C(38)-Ir(1)-Na(1)	96.67(8)
C(39)-C(40)	1.510(4)	C(39)-Ir(1)-Na(1)	118.33(7)
C(40)-C(41)	1.537(4)	O(1)-Ir(1)-Na(1)	38.13(5)
C(41)-C(42)	1.497(4)	C(42)-Ir(1)-Na(1)	159.57(8)
C(42)-C(43)	1.403(4)	N(1)-Ir(1)-Na(1)	72.25(5)
C(43)-C(44)	1.513(4)	C(43)-Ir(1)-Na(1)	131.26(8)
C(44)-C(45)	1.523(4)	O(2)-Na(1)-O(1)	104.80(7)
O(50)-C(51B)	1.4496(10)	O(2)-Na(1)-O(2)#1	100.48(7)
O(50)-C(51B)#2	1.4496(10)	O(1)-Na(1)-O(2)#1	106.99(7)
O(50)-C(51A)	1.4506(10)	O(2)-Na(1)-Na(1)#1	51.65(6)
O(50)-C(51A)#2	1.4507(10)	O(1)-Na(1)-Na(1)#1	115.38(7)
C(51A)-C(52A)	1.5498(10)	O(2)#1-Na(1)-Na(1)#1	48.84(5)
C(51B)-C(52B)	1.5527(10)	O(2)-Na(1)-Ir(1)	70.53(5)
		O(1)-Na(1)-Ir(1)	35.83(5)
C(38)-Ir(1)-C(39)	39.46(10)	O(2)#1-Na(1)-Ir(1)	123.00(6)
C(38)-Ir(1)-O(1)	91.52(9)	Na(1)#1-Na(1)-Ir(1)	100.32(5)
C(39)-Ir(1)-O(1)	90.96(8)	C(1)-O(1)-Ir(1)	108.76(14)
C(38)-Ir(1)-C(42)	97.80(11)	C(1)-O(1)-Na(1)	128.81(15)
C(39)-Ir(1)-C(42)	81.82(10)	Ir(1)-O(1)-Na(1)	106.04(8)
O(1)-Ir(1)-C(42)	154.83(9)	C(17)-O(2)-Na(1)	147.04(15)
C(38)-Ir(1)-N(1)	168.64(9)	C(17)-O(2)-Na(1)#1	123.32(15)
C(39)-Ir(1)-N(1)	148.52(9)	Na(1)-O(2)-Na(1)#1	79.52(7)
O(1)-Ir(1)-N(1)	81.27(7)	C(7)-N(1)-C(11)	119.3(2)
C(42)-Ir(1)-N(1)	92.35(9)	C(7)-N(1)-Ir(1)	114.54(15)
C(38)-Ir(1)-C(43)	80.45(10)	C(11)-N(1)-Ir(1)	126.05(15)
C(39)-Ir(1)-C(43)	89.89(10)	O(1)-C(1)-C(6)	120.4(2)
O(1)-Ir(1)-C(43)	166.20(9)	O(1)-C(1)-C(2)	121.1(2)

C(6)-C(1)-C(2)	118.6(2)	C(12)-C(13)-C(14)	121.5(2)
C(3)-C(2)-C(1)	117.2(2)	C(13)-C(14)-C(15)	115.7(2)
C(3)-C(2)-C(18)	120.6(2)	C(13)-C(14)-C(30)	120.8(2)
C(1)-C(2)-C(18)	122.2(2)	C(15)-C(14)-C(30)	123.4(2)
C(2)-C(3)-C(4)	124.5(2)	C(16)-C(15)-C(14)	124.8(2)
C(5)-C(4)-C(3)	116.4(2)	C(15)-C(16)-C(17)	118.7(2)
C(5)-C(4)-C(22)	123.2(2)	C(15)-C(16)-C(34)	119.6(2)
C(3)-C(4)-C(22)	120.4(2)	C(17)-C(16)-C(34)	121.7(2)
C(4)-C(5)-C(6)	122.4(2)	O(2)-C(17)-C(12)	119.3(2)
C(5)-C(6)-C(1)	120.1(2)	O(2)-C(17)-C(16)	124.6(2)
C(5)-C(6)-C(7)	118.3(2)	C(12)-C(17)-C(16)	116.1(2)
C(1)-C(6)-C(7)	121.0(2)	C(20)-C(18)-C(19)	107.1(2)
N(1)-C(7)-C(8)	120.6(2)	C(20)-C(18)-C(21)	107.9(2)
N(1)-C(7)-C(6)	120.8(2)	C(19)-C(18)-C(21)	109.7(2)
C(8)-C(7)-C(6)	118.5(2)	C(20)-C(18)-C(2)	111.5(2)
C(9)-C(8)-C(7)	121.5(2)	C(19)-C(18)-C(2)	111.7(2)
C(10)-C(9)-C(8)	116.1(2)	C(21)-C(18)-C(2)	108.85(19)
C(10)-C(9)-C(26)	121.4(2)	C(24)-C(22)-C(4)	111.0(2)
C(8)-C(9)-C(26)	122.5(2)	C(24)-C(22)-C(25)	107.8(2)
C(11)-C(10)-C(9)	121.5(2)	C(4)-C(22)-C(25)	111.9(2)
N(1)-C(11)-C(10)	120.8(2)	C(24)-C(22)-C(23)	109.2(2)
N(1)-C(11)-C(12)	117.0(2)	C(4)-C(22)-C(23)	108.6(2)
C(10)-C(11)-C(12)	122.2(2)	C(25)-C(22)-C(23)	108.3(2)
N(1)-C(11)-Na(1)#1	94.53(13)	C(27)-C(26)-C(29)	108.0(2)
C(10)-C(11)-Na(1)#1	83.37(13)	C(27)-C(26)-C(9)	112.6(2)
C(12)-C(11)-Na(1)#1	92.40(13)	C(29)-C(26)-C(9)	108.25(19)
C(13)-C(12)-C(17)	122.3(2)	C(27)-C(26)-C(28)	109.2(2)
C(13)-C(12)-C(11)	119.6(2)	C(29)-C(26)-C(28)	109.7(2)
C(17)-C(12)-C(11)	118.1(2)	C(9)-C(26)-C(28)	109.0(2)

C(14)-C(30)-C(32)	112.5(2)	C(51B)-O(50)-C(51A)	46.3(6)
C(14)-C(30)-C(31)	109.4(2)	C(51B)#2-O(50)-C(51A)	136.3(9)
C(32)-C(30)-C(31)	108.4(2)	C(51B)-O(50)-C(51A)#2	136.3(9)
C(14)-C(30)-C(33)	109.2(2)	C(51B)#2-O(50)-C(51A)#2	46.3(6)
C(32)-C(30)-C(33)	107.6(2)	C(51A)-O(50)-C(51A)#2	177.0(14)
C(31)-C(30)-C(33)	109.8(2)	O(50)-C(51A)-C(52A)	109.45(10)
C(36)-C(34)-C(35)	108.7(2)	O(50)-C(51B)-C(52B)	109.30(10)
C(36)-C(34)-C(16)	111.4(2)		
C(35)-C(34)-C(16)	108.9(2)		
C(36)-C(34)-C(37)	106.7(2)		
C(35)-C(34)-C(37)	108.8(2)		
C(16)-C(34)-C(37)	112.1(2)		
C(39)-C(38)-C(45)	123.4(2)		
C(39)-C(38)-Ir(1)	70.34(15)		
C(45)-C(38)-Ir(1)	114.80(19)		
C(38)-C(39)-C(40)	122.8(2)		
C(38)-C(39)-Ir(1)	70.20(14)		
C(40)-C(39)-Ir(1)	114.34(18)		
C(39)-C(40)-C(41)	110.8(2)		
C(42)-C(41)-C(40)	112.2(2)		
C(43)-C(42)-C(41)	125.6(3)		
C(43)-C(42)-Ir(1)	71.90(14)		
C(41)-C(42)-Ir(1)	110.65(18)		
C(42)-C(43)-C(44)	123.3(2)		
C(42)-C(43)-Ir(1)	69.39(14)		
C(44)-C(43)-Ir(1)	114.35(18)		
C(43)-C(44)-C(45)	112.7(2)		
C(38)-C(45)-C(44)	111.3(2)		
C(51B)-O(50)-C(51B)#2	104.2(8)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2

#2 -x+1,y,-z+1/2

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	188(1)	121(1)	134(1)	6(1)	107(1)	18(1)
Na(1)	211(5)	190(5)	320(6)	45(5)	121(5)	18(4)
O(1)	195(8)	139(8)	132(8)	4(6)	80(7)	8(6)
O(2)	157(8)	173(9)	179(9)	52(7)	74(7)	35(7)
N(1)	191(9)	98(8)	121(9)	0(7)	110(8)	-2(7)
C(1)	177(10)	130(10)	135(11)	3(9)	101(9)	7(8)
C(2)	183(10)	157(11)	105(10)	19(9)	103(9)	7(9)
C(3)	177(11)	147(10)	147(11)	45(9)	117(9)	15(9)
C(4)	136(10)	132(10)	138(11)	19(8)	85(9)	11(8)
C(5)	153(10)	125(10)	101(10)	9(8)	86(9)	24(8)
C(6)	190(10)	111(10)	107(10)	1(8)	109(9)	6(8)
C(7)	168(10)	110(10)	110(10)	3(8)	80(9)	4(8)
C(8)	184(10)	106(10)	114(11)	3(8)	81(9)	12(8)
C(9)	164(10)	141(11)	103(10)	4(8)	77(9)	26(8)
C(10)	177(10)	132(10)	122(11)	20(8)	106(9)	4(8)
C(11)	133(9)	121(10)	123(10)	18(8)	81(8)	17(8)
C(12)	139(10)	107(10)	135(11)	6(8)	106(9)	-4(8)
C(13)	150(10)	142(10)	100(10)	-8(8)	77(9)	-7(8)
C(14)	187(11)	126(10)	125(11)	25(9)	97(9)	6(8)
C(15)	202(11)	108(10)	164(12)	-15(9)	108(10)	-33(9)

C(16)	132(10)	165(11)	118(11)	-8(9)	76(9)	-26(8)
C(17)	140(10)	143(10)	135(11)	29(9)	99(9)	4(8)
C(18)	196(11)	187(12)	107(11)	19(9)	92(9)	-9(9)
C(19)	484(18)	373(17)	116(13)	-6(12)	117(13)	128(14)
C(20)	392(16)	338(16)	119(12)	63(11)	66(12)	-99(13)
C(21)	211(12)	530(20)	176(13)	53(13)	87(11)	-10(13)
C(22)	197(11)	170(11)	172(12)	13(9)	108(10)	-36(9)
C(23)	275(14)	346(16)	352(17)	-55(13)	214(13)	-125(12)
C(24)	350(15)	158(12)	307(16)	24(11)	144(13)	-20(11)
C(25)	284(13)	228(13)	200(14)	-14(11)	94(11)	-111(11)
C(26)	252(12)	178(11)	121(11)	0(9)	137(10)	43(10)
C(27)	363(14)	193(12)	180(13)	-67(10)	184(12)	-10(11)
C(28)	319(14)	225(13)	223(14)	18(11)	217(12)	56(11)
C(29)	322(14)	302(14)	115(12)	12(10)	134(11)	88(11)
C(30)	297(13)	132(11)	156(12)	23(9)	97(11)	21(10)
C(31)	259(14)	258(15)	307(16)	49(13)	48(12)	84(12)
C(32)	436(17)	121(12)	252(15)	48(11)	136(13)	19(11)
C(33)	650(20)	224(14)	183(14)	83(11)	220(15)	77(14)
C(34)	143(10)	188(12)	141(11)	-26(9)	54(9)	-31(9)
C(35)	165(11)	304(15)	260(14)	-57(12)	75(11)	-42(11)
C(36)	248(13)	281(14)	187(13)	-83(11)	86(11)	-5(11)
C(37)	301(14)	310(15)	134(12)	-14(11)	67(11)	-51(12)
C(38)	298(13)	206(12)	244(14)	-24(11)	206(12)	30(11)
C(39)	251(12)	237(13)	208(13)	45(11)	182(11)	48(10)
C(40)	261(13)	337(16)	365(17)	89(13)	216(13)	49(12)
C(41)	229(13)	369(17)	258(15)	32(13)	109(12)	29(12)
C(42)	243(12)	237(13)	162(12)	69(10)	102(10)	104(10)
C(43)	327(14)	179(12)	279(14)	103(11)	230(12)	111(11)
C(44)	386(16)	174(13)	394(17)	17(12)	292(14)	53(11)

C(45) 395(16) 222(14) 378(18) -79(13) 275(15) 3(12)

$[Ir(cod)]_2(ONO^{tBu})$, 5

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

This crystal is a twin and was integrated as such, with the minor component comprising 21.2%. Two bonded atoms (C51 and C52) had the anisotropic displacement parameters constrained to be equal so as to reduce the tendency of C51 to refine to unrealistic values.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	1173(1)	7712(1)	797(1)	13(1)
Ir(2)	4115(1)	7771(1)	1684(1)	13(1)
O(1)	2808(2)	8342(1)	1197(1)	14(1)
O(2)	3194(2)	7207(1)	1060(1)	13(1)
N(1)	1017(3)	7564(1)	1688(1)	12(1)
C(1)	2011(3)	8789(1)	1411(1)	14(1)
C(2)	2170(3)	9388(1)	1223(1)	17(1)
C(3)	1243(4)	9812(1)	1444(1)	21(1)
C(4)	214(3)	9691(1)	1840(1)	19(1)
C(5)	117(3)	9098(1)	2031(1)	16(1)
C(6)	974(3)	8652(1)	1819(1)	14(1)
C(7)	840(3)	8033(1)	2055(1)	12(1)

C(8)	564(3)	7933(1)	2632(1)	13(1)
C(9)	490(3)	7355(1)	2859(1)	14(1)
C(10)	855(3)	6892(1)	2483(1)	14(1)
C(11)	1148(3)	6999(1)	1907(1)	14(1)
C(12)	1690(3)	6517(1)	1526(1)	15(1)
C(13)	1181(4)	5936(1)	1597(1)	18(1)
C(14)	1751(4)	5456(1)	1298(1)	22(1)
C(15)	2854(4)	5580(1)	946(1)	24(1)
C(16)	3418(4)	6153(1)	852(1)	19(1)
C(17)	2786(3)	6632(1)	1144(1)	15(1)
C(18)	3219(4)	9620(1)	783(1)	23(1)
C(19)	2397(4)	9860(2)	243(2)	36(1)
C(20)	4074(4)	10136(1)	1068(2)	34(1)
C(21)	4286(4)	9164(1)	563(1)	25(1)
C(22)	-806(4)	10169(1)	2055(2)	26(1)
C(23)	-490(5)	10791(2)	1829(2)	62(2)
C(24)	-672(6)	10214(2)	2726(2)	70(2)
C(25)	-2267(5)	10003(2)	1883(3)	62(2)
C(26)	105(3)	7225(1)	3487(1)	20(1)
C(27)	1419(4)	7043(2)	3841(1)	37(1)
C(28)	-969(4)	6716(1)	3499(1)	26(1)
C(29)	-543(5)	7774(1)	3769(1)	38(1)
C(30)	1192(5)	4814(1)	1350(2)	32(1)
C(31)	2436(5)	4391(2)	1537(3)	60(2)
C(32)	614(7)	4611(2)	752(2)	83(2)
C(33)	114(5)	4749(1)	1803(2)	44(1)
C(34)	4670(4)	6190(1)	443(1)	24(1)
C(35)	4201(5)	5939(1)	-157(1)	38(1)
C(36)	5274(4)	6816(1)	338(1)	22(1)

C(37)	5890(4)	5811(1)	708(2)	39(1)
C(38)	-940(4)	7911(1)	707(1)	22(1)
C(39)	-690(3)	7286(1)	578(1)	20(1)
C(40)	-814(4)	7036(1)	-40(1)	31(1)
C(41)	606(4)	7052(2)	-330(2)	39(1)
C(42)	1537(4)	7547(2)	-85(1)	32(1)
C(43)	1133(4)	8148(2)	-29(1)	36(1)
C(44)	-299(5)	8385(2)	-234(2)	40(1)
C(45)	-1309(4)	8388(1)	267(2)	37(1)
C(46)	4311(3)	8308(1)	2425(1)	19(1)
C(47)	4521(4)	7972(1)	2983(1)	26(1)
C(48)	4635(4)	7301(1)	2906(1)	31(1)
C(49)	4688(4)	7102(1)	2286(1)	22(1)
C(50)	5860(5)	7249(2)	1931(2)	50(1)
C(51)	7087(5)	7666(3)	2205(2)	70(1)
C(52)	6858(5)	8303(3)	2150(2)	70(1)
C(53)	5381(5)	8438(2)	2048(2)	39(1)

Table S7. Selected bond lengths [Å] and angles [°] for **5**.

Ir(1)-C(39)	2.064(3)	C(39)-Ir(1)-C(38)	41.03(11)
Ir(1)-C(38)	2.069(3)	C(39)-Ir(1)-N(1)	94.20(10)
Ir(1)-N(1)	2.082(2)	C(38)-Ir(1)-N(1)	91.59(10)
Ir(1)-C(42)	2.098(3)	C(39)-Ir(1)-C(42)	81.72(13)
Ir(1)-C(43)	2.127(3)	C(38)-Ir(1)-C(42)	97.84(13)
Ir(1)-O(1)	2.2701(19)	N(1)-Ir(1)-C(42)	159.96(11)
Ir(1)-O(2)	2.2962(19)	C(39)-Ir(1)-C(43)	90.38(12)
Ir(2)-C(53)	2.075(3)	C(38)-Ir(1)-C(43)	80.04(14)
Ir(2)-O(2)	2.0771(17)	N(1)-Ir(1)-C(43)	161.31(12)
Ir(2)-O(1)	2.0808(18)	C(42)-Ir(1)-C(43)	38.73(14)
Ir(2)-C(46)	2.084(3)	C(39)-Ir(1)-O(1)	163.38(10)
Ir(2)-C(49)	2.092(3)	C(38)-Ir(1)-O(1)	124.14(9)
Ir(2)-C(50)	2.094(4)	N(1)-Ir(1)-O(1)	76.96(8)
		C(42)-Ir(1)-O(1)	111.31(11)
		C(43)-Ir(1)-O(1)	93.85(10)
		C(39)-Ir(1)-O(2)	123.08(9)
		C(38)-Ir(1)-O(2)	159.82(9)
		N(1)-Ir(1)-O(2)	75.75(8)
		C(42)-Ir(1)-O(2)	89.99(12)
		C(43)-Ir(1)-O(2)	116.46(13)
		O(1)-Ir(1)-O(2)	68.86(6)
		C(53)-Ir(2)-O(2)	159.81(11)
		C(53)-Ir(2)-O(1)	96.00(13)
		O(2)-Ir(2)-O(1)	76.77(7)
		C(53)-Ir(2)-C(46)	39.11(14)
		O(2)-Ir(2)-C(46)	159.08(11)
		O(1)-Ir(2)-C(46)	96.78(9)

C(53)-Ir(2)-C(49)	96.40(13)	O(2)-Ir(2)-C(50)	99.39(13)
O(2)-Ir(2)-C(49)	96.74(9)	O(1)-Ir(2)-C(50)	160.44(13)
O(1)-Ir(2)-C(49)	158.20(11)	C(46)-Ir(2)-C(50)	93.00(14)
C(46)-Ir(2)-C(49)	81.85(11)	C(49)-Ir(2)-C(50)	40.38(15)
C(53)-Ir(2)-C(50)	81.04(19)		

Table S8. Bond lengths [Å] and angles [°] for **5**.

Ir(1)-C(39)	2.064(3)	C(4)-C(5)	1.397(4)
Ir(1)-C(38)	2.069(3)	C(4)-C(22)	1.538(4)
Ir(1)-N(1)	2.082(2)	C(5)-C(6)	1.387(4)
Ir(1)-C(42)	2.098(3)	C(6)-C(7)	1.491(3)
Ir(1)-C(43)	2.127(3)	C(7)-C(8)	1.376(4)
Ir(1)-O(1)	2.2701(19)	C(8)-C(9)	1.393(3)
Ir(1)-O(2)	2.2962(19)	C(9)-C(10)	1.398(3)
Ir(2)-C(53)	2.075(3)	C(9)-C(26)	1.528(4)
Ir(2)-O(2)	2.0771(17)	C(10)-C(11)	1.380(4)
Ir(2)-O(1)	2.0808(18)	C(11)-C(12)	1.491(4)
Ir(2)-C(46)	2.084(3)	C(12)-C(13)	1.397(3)
Ir(2)-C(49)	2.092(3)	C(12)-C(17)	1.413(4)
Ir(2)-C(50)	2.094(4)	C(13)-C(14)	1.393(4)
O(1)-C(1)	1.356(3)	C(14)-C(15)	1.380(5)
O(2)-C(17)	1.357(3)	C(14)-C(30)	1.535(4)
N(1)-C(7)	1.359(3)	C(15)-C(16)	1.408(4)
N(1)-C(11)	1.361(3)	C(16)-C(17)	1.407(4)
C(1)-C(2)	1.416(3)	C(16)-C(34)	1.548(4)
C(1)-C(6)	1.422(4)	C(18)-C(19)	1.537(5)
C(2)-C(3)	1.404(4)	C(18)-C(21)	1.538(4)
C(2)-C(18)	1.537(4)	C(18)-C(20)	1.543(4)
C(3)-C(4)	1.387(5)	C(22)-C(25)	1.483(6)

C(22)-C(23)	1.515(5)	C(39)-Ir(1)-N(1)	94.20(10)
C(22)-C(24)	1.544(6)	C(38)-Ir(1)-N(1)	91.59(10)
C(26)-C(27)	1.525(5)	C(39)-Ir(1)-C(42)	81.72(13)
C(26)-C(29)	1.529(4)	C(38)-Ir(1)-C(42)	97.84(13)
C(26)-C(28)	1.532(4)	N(1)-Ir(1)-C(42)	159.96(11)
C(30)-C(33)	1.496(5)	C(39)-Ir(1)-C(43)	90.38(12)
C(30)-C(32)	1.529(6)	C(38)-Ir(1)-C(43)	80.04(14)
C(30)-C(31)	1.563(6)	N(1)-Ir(1)-C(43)	161.31(12)
C(34)-C(36)	1.534(4)	C(42)-Ir(1)-C(43)	38.73(14)
C(34)-C(35)	1.538(4)	C(39)-Ir(1)-O(1)	163.38(10)
C(34)-C(37)	1.546(5)	C(38)-Ir(1)-O(1)	124.14(9)
C(38)-C(39)	1.449(4)	N(1)-Ir(1)-O(1)	76.96(8)
C(38)-C(45)	1.500(4)	C(42)-Ir(1)-O(1)	111.31(11)
C(39)-C(40)	1.524(4)	C(43)-Ir(1)-O(1)	93.85(10)
C(40)-C(41)	1.533(5)	C(39)-Ir(1)-O(2)	123.08(9)
C(41)-C(42)	1.515(5)	C(38)-Ir(1)-O(2)	159.82(9)
C(42)-C(43)	1.401(5)	N(1)-Ir(1)-O(2)	75.75(8)
C(43)-C(44)	1.525(5)	C(42)-Ir(1)-O(2)	89.99(12)
C(44)-C(45)	1.527(6)	C(43)-Ir(1)-O(2)	116.46(13)
C(46)-C(53)	1.392(5)	O(1)-Ir(1)-O(2)	68.86(6)
C(46)-C(47)	1.492(4)	C(53)-Ir(2)-O(2)	159.81(11)
C(47)-C(48)	1.511(4)	C(53)-Ir(2)-O(1)	96.00(13)
C(48)-C(49)	1.493(4)	O(2)-Ir(2)-O(1)	76.77(7)
C(49)-C(50)	1.445(6)	C(53)-Ir(2)-C(46)	39.11(14)
C(50)-C(51)	1.606(6)	O(2)-Ir(2)-C(46)	159.08(11)
C(51)-C(52)	1.443(7)	O(1)-Ir(2)-C(46)	96.78(9)
C(52)-C(53)	1.454(6)	C(53)-Ir(2)-C(49)	96.40(13)
		O(2)-Ir(2)-C(49)	96.74(9)
C(39)-Ir(1)-C(38)	41.03(11)	O(1)-Ir(2)-C(49)	158.20(11)

C(46)-Ir(2)-C(49)	81.85(11)	N(1)-C(7)-C(8)	120.1(2)
C(53)-Ir(2)-C(50)	81.04(19)	N(1)-C(7)-C(6)	118.4(2)
O(2)-Ir(2)-C(50)	99.39(13)	C(8)-C(7)-C(6)	121.5(2)
O(1)-Ir(2)-C(50)	160.44(13)	C(7)-C(8)-C(9)	121.6(2)
C(46)-Ir(2)-C(50)	93.00(14)	C(8)-C(9)-C(10)	115.9(2)
C(49)-Ir(2)-C(50)	40.38(15)	C(8)-C(9)-C(26)	123.1(2)
C(1)-O(1)-Ir(2)	126.21(16)	C(10)-C(9)-C(26)	120.9(2)
C(1)-O(1)-Ir(1)	102.38(16)	C(11)-C(10)-C(9)	121.7(2)
Ir(2)-O(1)-Ir(1)	103.13(7)	N(1)-C(11)-C(10)	119.7(2)
C(17)-O(2)-Ir(2)	126.27(15)	N(1)-C(11)-C(12)	118.7(2)
C(17)-O(2)-Ir(1)	105.03(17)	C(10)-C(11)-C(12)	121.5(2)
Ir(2)-O(2)-Ir(1)	102.37(7)	C(13)-C(12)-C(17)	120.6(2)
C(7)-N(1)-C(11)	119.8(2)	C(13)-C(12)-C(11)	118.2(3)
C(7)-N(1)-Ir(1)	120.05(16)	C(17)-C(12)-C(11)	121.0(2)
C(11)-N(1)-Ir(1)	120.10(16)	C(14)-C(13)-C(12)	120.9(3)
O(1)-C(1)-C(2)	121.1(3)	C(15)-C(14)-C(13)	117.0(2)
O(1)-C(1)-C(6)	119.7(2)	C(15)-C(14)-C(30)	120.5(3)
C(2)-C(1)-C(6)	119.2(2)	C(13)-C(14)-C(30)	122.5(3)
C(3)-C(2)-C(1)	116.7(3)	C(14)-C(15)-C(16)	125.2(3)
C(3)-C(2)-C(18)	116.5(2)	C(15)-C(16)-C(17)	116.3(3)
C(1)-C(2)-C(18)	126.7(3)	C(15)-C(16)-C(34)	116.7(2)
C(4)-C(3)-C(2)	125.2(2)	C(17)-C(16)-C(34)	127.0(2)
C(3)-C(4)-C(5)	116.5(3)	O(2)-C(17)-C(16)	121.3(3)
C(3)-C(4)-C(22)	123.1(2)	O(2)-C(17)-C(12)	118.8(2)
C(5)-C(4)-C(22)	120.4(3)	C(16)-C(17)-C(12)	119.9(2)
C(6)-C(5)-C(4)	121.5(3)	C(19)-C(18)-C(21)	107.0(3)
C(5)-C(6)-C(1)	120.7(2)	C(19)-C(18)-C(2)	108.6(3)
C(5)-C(6)-C(7)	118.6(3)	C(21)-C(18)-C(2)	116.6(2)
C(1)-C(6)-C(7)	120.6(2)	C(19)-C(18)-C(20)	109.1(3)

C(21)-C(18)-C(20)	106.7(3)	C(38)-C(39)-C(40)	122.3(2)
C(2)-C(18)-C(20)	108.7(3)	C(38)-C(39)-Ir(1)	69.68(18)
C(25)-C(22)-C(23)	109.6(4)	C(40)-C(39)-Ir(1)	115.6(2)
C(25)-C(22)-C(4)	110.0(3)	C(39)-C(40)-C(41)	110.8(3)
C(23)-C(22)-C(4)	112.9(3)	C(42)-C(41)-C(40)	111.8(3)
C(25)-C(22)-C(24)	108.9(4)	C(43)-C(42)-C(41)	124.9(4)
C(23)-C(22)-C(24)	105.7(3)	C(43)-C(42)-Ir(1)	71.77(18)
C(4)-C(22)-C(24)	109.6(3)	C(41)-C(42)-Ir(1)	111.8(2)
C(27)-C(26)-C(9)	109.4(3)	C(42)-C(43)-C(44)	123.4(3)
C(27)-C(26)-C(29)	109.0(3)	C(42)-C(43)-Ir(1)	69.50(17)
C(9)-C(26)-C(29)	111.2(2)	C(44)-C(43)-Ir(1)	114.9(2)
C(27)-C(26)-C(28)	109.4(3)	C(43)-C(44)-C(45)	110.7(3)
C(9)-C(26)-C(28)	110.0(2)	C(38)-C(45)-C(44)	111.3(3)
C(29)-C(26)-C(28)	107.8(3)	C(53)-C(46)-C(47)	124.0(3)
C(33)-C(30)-C(32)	111.1(4)	C(53)-C(46)-Ir(2)	70.11(17)
C(33)-C(30)-C(14)	113.2(3)	C(47)-C(46)-Ir(2)	114.56(17)
C(32)-C(30)-C(14)	108.8(3)	C(46)-C(47)-C(48)	114.0(2)
C(33)-C(30)-C(31)	106.7(3)	C(49)-C(48)-C(47)	114.2(2)
C(32)-C(30)-C(31)	108.3(4)	C(50)-C(49)-C(48)	121.6(3)
C(14)-C(30)-C(31)	108.7(3)	C(50)-C(49)-Ir(2)	69.88(18)
C(36)-C(34)-C(35)	106.9(2)	C(48)-C(49)-Ir(2)	113.59(18)
C(36)-C(34)-C(37)	106.1(3)	C(49)-C(50)-C(51)	118.6(3)
C(35)-C(34)-C(37)	110.1(3)	C(49)-C(50)-Ir(2)	69.7(2)
C(36)-C(34)-C(16)	116.5(2)	C(51)-C(50)-Ir(2)	110.2(3)
C(35)-C(34)-C(16)	108.5(3)	C(52)-C(51)-C(50)	115.5(4)
C(37)-C(34)-C(16)	108.7(3)	C(53)-C(52)-C(51)	111.2(4)
C(39)-C(38)-C(45)	125.7(3)	C(46)-C(53)-C(52)	125.9(4)
C(39)-C(38)-Ir(1)	69.29(17)	C(46)-C(53)-Ir(2)	70.77(17)
C(45)-C(38)-Ir(1)	115.1(3)	C(52)-C(53)-Ir(2)	117.6(3)

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	150(1)	166(1)	87(1)	6(1)	11(1)	-26(1)
Ir(2)	116(1)	164(1)	123(1)	-10(1)	15(1)	2(1)
O(1)	140(12)	161(7)	113(8)	1(6)	10(8)	4(7)
O(2)	135(10)	134(7)	133(8)	-2(6)	27(7)	-6(8)
N(1)	101(13)	140(8)	135(10)	6(7)	17(9)	-3(8)
C(1)	141(16)	154(10)	139(12)	-5(8)	-16(11)	-10(10)
C(2)	158(16)	164(10)	186(13)	20(9)	-5(12)	-7(10)
C(3)	211(18)	137(10)	282(15)	17(9)	-10(14)	-3(11)
C(4)	155(17)	167(10)	240(14)	-17(9)	-7(12)	10(11)
C(5)	109(15)	195(11)	168(12)	-20(9)	5(11)	11(10)
C(6)	129(16)	144(9)	132(11)	-13(8)	11(10)	9(10)
C(7)	68(13)	155(9)	153(11)	-20(8)	3(10)	13(10)
C(8)	113(15)	165(9)	124(11)	-35(8)	25(10)	-21(10)
C(9)	118(14)	218(11)	100(10)	-25(8)	3(10)	-19(10)
C(10)	146(15)	160(9)	119(11)	10(8)	-1(11)	-22(10)
C(11)	120(15)	152(9)	137(11)	-13(8)	13(11)	-29(10)
C(12)	223(17)	120(9)	118(11)	6(8)	21(11)	6(10)
C(13)	248(18)	150(10)	156(12)	3(8)	54(12)	-47(11)
C(14)	350(20)	129(10)	200(13)	-9(9)	54(13)	-38(12)
C(15)	390(20)	136(10)	189(14)	-30(9)	89(14)	16(12)
C(16)	280(20)	162(10)	135(12)	4(8)	60(12)	10(11)
C(17)	174(17)	135(10)	137(12)	-9(8)	17(11)	-2(10)
C(18)	204(18)	178(11)	299(16)	67(10)	25(14)	-35(12)
C(19)	320(20)	435(18)	326(19)	170(15)	59(16)	15(17)

C(20)	280(20)	292(14)	470(20)	-14(13)	119(18)	-114(15)
C(21)	230(20)	251(12)	280(16)	57(11)	93(14)	-53(13)
C(22)	203(19)	200(12)	382(18)	-19(11)	38(15)	60(12)
C(23)	580(40)	248(15)	1060(40)	-27(19)	320(30)	99(19)
C(24)	1030(50)	610(30)	480(30)	-140(20)	40(30)	490(30)
C(25)	320(30)	430(20)	1090(50)	-160(20)	40(30)	110(20)
C(26)	224(17)	266(12)	102(11)	1(9)	51(10)	-34(13)
C(27)	300(20)	630(20)	167(15)	137(14)	-45(15)	-121(18)
C(28)	260(20)	334(14)	190(13)	41(11)	60(13)	-52(14)
C(29)	610(30)	347(15)	192(15)	-66(12)	193(16)	-33(18)
C(30)	530(30)	156(11)	290(16)	-9(10)	138(17)	-87(14)
C(31)	500(30)	241(16)	1090(40)	160(20)	360(30)	55(18)
C(32)	1570(60)	490(20)	440(30)	-143(19)	80(30)	-580(30)
C(33)	580(30)	179(12)	560(30)	11(13)	270(20)	-75(16)
C(34)	320(20)	169(11)	223(14)	14(9)	137(14)	40(12)
C(35)	630(30)	271(13)	252(16)	-85(11)	253(18)	-85(17)
C(36)	260(20)	235(12)	188(14)	6(10)	120(13)	17(13)
C(37)	370(30)	353(15)	470(20)	128(15)	221(19)	148(16)
C(38)	187(17)	364(14)	118(12)	0(10)	-51(12)	95(13)
C(39)	114(15)	310(13)	169(12)	31(10)	1(10)	-54(13)
C(40)	330(20)	338(14)	249(16)	-81(12)	-82(16)	-62(15)
C(41)	330(20)	620(20)	201(16)	-204(14)	-40(16)	82(18)
C(42)	202(19)	680(20)	101(13)	-3(13)	56(13)	-16(17)
C(43)	380(20)	522(19)	171(14)	155(13)	-56(15)	-239(18)
C(44)	510(30)	379(17)	303(19)	144(13)	-190(19)	-90(17)
C(45)	420(30)	375(16)	299(18)	-14(13)	-130(18)	125(17)
C(46)	212(18)	163(10)	200(13)	-63(9)	-57(12)	13(11)
C(47)	380(20)	232(12)	174(13)	-47(10)	53(14)	-80(13)
C(48)	370(20)	287(14)	271(16)	102(12)	90(14)	163(15)

C(49)	219(18)	125(10)	306(16)	8(9)	-78(14)	12(11)
C(50)	580(30)	720(30)	190(16)	68(16)	18(17)	440(30)
C(51)	210(17)	1450(30)	440(18)	180(20)	-7(14)	-200(20)
C(52)	210(17)	1450(30)	440(18)	180(20)	-7(14)	-200(20)
C(53)	460(30)	530(20)	181(15)	-49(13)	-9(16)	-352(19)

[(ONO^{tBu})Ir(cod)(MeCN)][PF$_6$], 6

Crystals were mounted on a glass fiber using Paratone oil, then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors (gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **6**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	6791(1)	6738(1)	7256(1)	10(1)
O(1)	7252(1)	7114(1)	8303(1)	13(1)
O(2)	6629(1)	6034(1)	6195(1)	13(1)
N(1)	5830(1)	5183(1)	7311(1)	11(1)
N(2)	8385(1)	5993(1)	7294(1)	13(1)
C(1)	6445(1)	6959(1)	8719(1)	12(1)
C(2)	6686(1)	7617(1)	9423(1)	14(1)
C(3)	5750(1)	7567(1)	9815(1)	16(1)

C(4)	4588(1)	6908(1)	9555(1)	16(1)
C(5)	4432(1)	6192(1)	8894(1)	15(1)
C(6)	5363(1)	6146(1)	8480(1)	12(1)
C(7)	5216(1)	5157(1)	7851(1)	11(1)
C(8)	4473(1)	4129(1)	7841(1)	13(1)
C(9)	4248(1)	3147(1)	7279(1)	11(1)
C(10)	4909(1)	3196(1)	6748(1)	12(1)
C(11)	5752(1)	4169(1)	6788(1)	11(1)
C(12)	6557(1)	4038(1)	6254(1)	11(1)
C(13)	6925(1)	2913(1)	6022(1)	13(1)
C(14)	7512(1)	2612(1)	5454(1)	13(1)
C(15)	7687(1)	3468(1)	5103(1)	14(1)
C(16)	7383(1)	4612(1)	5322(1)	12(1)
C(17)	6869(1)	4925(1)	5943(1)	11(1)
C(18)	7945(1)	8352(1)	9751(1)	16(1)
C(19)	8973(1)	7572(1)	9612(1)	22(1)
C(20)	8037(1)	8833(1)	10533(1)	23(1)
C(21)	8163(1)	9413(1)	9464(1)	23(1)
C(22)	3533(1)	6902(1)	9977(1)	24(1)
C(23)	3212(2)	5654(1)	10047(1)	47(1)
C(24)	2397(1)	7247(2)	9594(1)	44(1)
C(25)	3840(1)	7777(1)	10687(1)	34(1)
C(26)	3361(1)	2055(1)	7236(1)	14(1)
C(27)	4014(1)	956(1)	7041(1)	23(1)
C(28)	2257(1)	1968(1)	6683(1)	24(1)
C(29)	2891(1)	2102(1)	7913(1)	24(1)
C(30)	7910(1)	1377(1)	5231(1)	16(1)
C(31)	8848(1)	1211(1)	5808(1)	30(1)
C(32)	8492(1)	1184(1)	4576(1)	24(1)

C(33)	6783(1)	439(1)	5094(1)	21(1)
C(34)	7574(1)	5482(1)	4894(1)	14(1)
C(35)	8608(1)	6480(1)	5280(1)	19(1)
C(36)	6358(1)	5965(1)	4734(1)	18(1)
C(37)	7956(1)	4908(1)	4197(1)	20(1)
C(38)	5185(1)	7690(1)	7506(1)	14(1)
C(39)	5171(1)	7380(1)	6801(1)	15(1)
C(40)	5496(1)	8218(1)	6382(1)	19(1)
C(41)	6875(1)	8463(1)	6334(1)	19(1)
C(42)	7729(1)	8190(1)	6890(1)	16(1)
C(43)	7685(1)	8643(1)	7577(1)	16(1)
C(44)	6792(1)	9498(1)	7833(1)	18(1)
C(45)	5618(1)	8895(1)	7992(1)	17(1)
C(46)	9212(1)	5488(1)	7271(1)	16(1)
C(47)	10233(1)	4796(1)	7219(1)	31(1)
P(1)	1636(1)	8178(1)	7446(1)	22(1)
F(1)	695(1)	7257(1)	6836(1)	27(1)
F(2)	2215(1)	7093(1)	7645(1)	36(1)
F(3)	2614(1)	8199(1)	6930(1)	28(1)
F(4)	657(1)	8138(1)	7952(1)	46(1)
F(5)	1063(1)	9250(1)	7233(1)	43(1)
F(6)	2582(1)	9092(1)	8047(1)	42(1)
C(51)	7897(1)	3318(1)	7987(1)	30(1)
C(52)	8515(1)	2334(1)	7864(1)	31(1)
C(53)	9660(1)	2375(1)	8247(1)	32(1)
C(54)	10173(1)	3403(1)	8739(1)	31(1)
C(55)	9559(1)	4387(1)	8855(1)	30(1)

C(56)	8416(1)	4342(1)	8480(1)	28(1)

Table S11. Selected bond lengths [Å] and angles [°] for **6**.

Ir(1)-N(2)	2.0456(8)	N(2)-Ir(1)-O(1)	81.05(3)
Ir(1)-O(1)	2.0540(7)	N(2)-Ir(1)-N(1)	89.69(3)
Ir(1)-N(1)	2.0736(8)	O(1)-Ir(1)-N(1)	85.86(3)
Ir(1)-O(2)	2.0849(7)	N(2)-Ir(1)-O(2)	85.09(3)
Ir(1)-C(39)	2.2030(9)	O(1)-Ir(1)-O(2)	165.29(3)
Ir(1)-C(38)	2.2322(9)	N(1)-Ir(1)-O(2)	89.17(3)
Ir(1)-C(42)	2.2612(10)	N(2)-Ir(1)-C(39)	158.10(4)
Ir(1)-C(43)	2.2660(9)	O(1)-Ir(1)-C(39)	120.57(3)
		N(1)-Ir(1)-C(39)	95.01(3)
		O(2)-Ir(1)-C(39)	73.63(3)
		N(2)-Ir(1)-C(38)	165.27(3)
		O(1)-Ir(1)-C(38)	84.25(3)
		N(1)-Ir(1)-C(38)	90.18(3)
		O(2)-Ir(1)-C(38)	109.63(3)
		C(39)-Ir(1)-C(38)	36.42(4)
		N(2)-Ir(1)-C(42)	89.93(3)
		O(1)-Ir(1)-C(42)	109.25(3)
		N(1)-Ir(1)-C(42)	164.63(3)
		O(2)-Ir(1)-C(42)	75.49(3)
		C(39)-Ir(1)-C(42)	79.95(4)
		C(38)-Ir(1)-C(42)	94.05(4)
		N(2)-Ir(1)-C(43)	96.56(3)
		O(1)-Ir(1)-C(43)	76.08(3)
		N(1)-Ir(1)-C(43)	159.65(3)
		O(2)-Ir(1)-C(43)	110.60(3)
		C(39)-Ir(1)-C(43)	86.38(4)

C(38)-Ir(1)-C(43)	78.90(4)	C(42)-Ir(1)-C(43)	35.32(4)

Table S12. Bond lengths [Å] and angles [°] for **6**.

Ir(1)-N(2)	2.0456(8)	C(7)-C(8)	1.3964(13)
Ir(1)-O(1)	2.0540(7)	C(8)-C(9)	1.3813(12)
Ir(1)-N(1)	2.0736(8)	C(8)-H(8)	0.940(12)
Ir(1)-O(2)	2.0849(7)	C(9)-C(10)	1.3915(13)
Ir(1)-C(39)	2.2030(9)	C(9)-C(26)	1.5235(12)
Ir(1)-C(38)	2.2322(9)	C(10)-C(11)	1.3890(12)
Ir(1)-C(42)	2.2612(10)	C(10)-H(10)	0.943(12)
Ir(1)-C(43)	2.2660(9)	C(11)-C(12)	1.4785(12)
O(1)-C(1)	1.3381(11)	C(12)-C(17)	1.4002(13)
O(2)-C(17)	1.3430(11)	C(12)-C(13)	1.4066(12)
N(1)-C(11)	1.3693(11)	C(13)-C(14)	1.3827(13)
N(1)-C(7)	1.3700(11)	C(13)-H(13)	0.935(12)
N(2)-C(46)	1.1371(12)	C(14)-C(15)	1.3974(14)
C(1)-C(6)	1.4108(12)	C(14)-C(30)	1.5353(13)
C(1)-C(2)	1.4240(13)	C(15)-C(16)	1.3968(13)
C(2)-C(3)	1.3920(13)	C(15)-H(15)	0.923(11)
C(2)-C(18)	1.5425(13)	C(16)-C(17)	1.4282(12)
C(3)-C(4)	1.4020(13)	C(16)-C(34)	1.5318(13)
C(3)-H(3)	0.894(13)	C(18)-C(21)	1.5307(16)
C(4)-C(5)	1.3740(13)	C(18)-C(19)	1.5375(14)
C(4)-C(22)	1.5342(13)	C(18)-C(20)	1.5348(14)
C(5)-C(6)	1.4083(12)	C(19)-H(19A)	0.929(14)
C(5)-H(5)	0.950(11)	C(19)-H(19B)	0.971(14)
C(6)-C(7)	1.4732(12)	C(19)-H(19C)	0.975(13)

C(20)-H(20A)	0.978(13)	C(29)-H(29C)	0.945(15)
C(20)-H(20B)	0.998(14)	C(30)-C(32)	1.5275(15)
C(20)-H(20C)	0.964(12)	C(30)-C(33)	1.5354(14)
C(21)-H(21A)	0.981(15)	C(30)-C(31)	1.5353(16)
C(21)-H(21B)	0.997(13)	C(31)-H(31A)	0.956(16)
C(21)-H(21C)	0.924(14)	C(31)-H(31B)	0.994(14)
C(22)-C(25)	1.5220(16)	C(31)-H(31C)	0.950(15)
C(22)-C(23)	1.533(2)	C(32)-H(32A)	0.944(13)
C(22)-C(24)	1.5416(19)	C(32)-H(32B)	0.964(14)
C(23)-H(23A)	1.090(18)	C(32)-H(32C)	0.986(14)
C(23)-H(23B)	1.060(18)	C(33)-H(33A)	0.988(13)
C(23)-H(23C)	1.036(15)	C(33)-H(33B)	0.965(13)
C(24)-H(24A)	0.938(18)	C(33)-H(33C)	0.927(14)
C(24)-H(24B)	0.978(15)	C(34)-C(37)	1.5371(14)
C(24)-H(24C)	1.039(18)	C(34)-C(36)	1.5412(13)
C(25)-H(25A)	0.997(14)	C(34)-C(35)	1.5351(14)
C(25)-H(25B)	0.987(16)	C(35)-H(35A)	0.923(14)
C(25)-H(25C)	0.972(18)	C(35)-H(35B)	0.989(15)
C(26)-C(29)	1.5271(14)	C(35)-H(35C)	0.989(12)
C(26)-C(27)	1.5325(14)	C(36)-H(36A)	0.946(12)
C(26)-C(28)	1.5316(14)	C(36)-H(36B)	0.935(14)
C(27)-H(27A)	0.953(15)	C(36)-H(36C)	0.994(12)
C(27)-H(27B)	0.955(14)	C(37)-H(37A)	0.957(12)
C(27)-H(27C)	0.946(14)	C(37)-H(37B)	0.972(14)
C(28)-H(28A)	0.964(15)	C(37)-H(37C)	0.984(12)
C(28)-H(28B)	0.995(16)	C(38)-C(39)	1.3863(14)
C(28)-H(28C)	0.947(15)	C(38)-C(45)	1.5041(13)
C(29)-H(29A)	0.950(15)	C(38)-H(38)	0.948(12)
C(29)-H(29B)	0.910(14)	C(39)-C(40)	1.5160(15)

C(39)-H(39)	0.959(11)	C(52)-C(53)	1.3930(18)
C(40)-C(41)	1.5453(15)	C(52)-H(52)	0.955(15)
C(40)-H(40A)	0.971(12)	C(53)-C(54)	1.3790(19)
C(40)-H(40B)	0.965(12)	C(53)-H(53)	0.892(15)
C(41)-C(42)	1.5061(15)	C(54)-C(55)	1.3835(18)
C(41)-H(41A)	0.943(12)	C(54)-H(54)	0.973(13)
C(41)-H(41B)	0.963(13)	C(55)-C(56)	1.3835(17)
C(42)-C(43)	1.3735(14)	C(55)-H(55)	0.976(15)
C(42)-H(42)	0.944(11)	C(56)-H(56)	0.939(13)
C(43)-C(44)	1.5192(14)		
C(43)-H(43)	0.923(11)	N(2)-Ir(1)-O(1)	81.05(3)
C(44)-C(45)	1.5340(14)	N(2)-Ir(1)-N(1)	89.69(3)
C(44)-H(44A)	0.973(13)	O(1)-Ir(1)-N(1)	85.86(3)
C(44)-H(44B)	0.958(13)	N(2)-Ir(1)-O(2)	85.09(3)
C(45)-H(45A)	0.944(12)	O(1)-Ir(1)-O(2)	165.29(3)
C(45)-H(45B)	0.981(13)	N(1)-Ir(1)-O(2)	89.17(3)
C(46)-C(47)	1.4541(14)	N(2)-Ir(1)-C(39)	158.10(4)
C(47)-H(47A)	0.89(2)	O(1)-Ir(1)-C(39)	120.57(3)
C(47)-H(47B)	0.93(2)	N(1)-Ir(1)-C(39)	95.01(3)
C(47)-H(47C)	1.01(3)	O(2)-Ir(1)-C(39)	73.63(3)
P(1)-F(4)	1.5938(8)	N(2)-Ir(1)-C(38)	165.27(3)
P(1)-F(5)	1.6034(8)	O(1)-Ir(1)-C(38)	84.25(3)
P(1)-F(1)	1.6055(7)	N(1)-Ir(1)-C(38)	90.18(3)
P(1)-F(3)	1.6033(7)	O(2)-Ir(1)-C(38)	109.63(3)
P(1)-F(6)	1.5948(7)	C(39)-Ir(1)-C(38)	36.42(4)
P(1)-F(2)	1.6082(8)	N(2)-Ir(1)-C(42)	89.93(3)
C(51)-C(52)	1.3864(19)	O(1)-Ir(1)-C(42)	109.25(3)
C(51)-C(56)	1.3780(19)	N(1)-Ir(1)-C(42)	164.63(3)
C(51)-H(51)	0.942(14)	O(2)-Ir(1)-C(42)	75.49(3)

C(39)-Ir(1)-C(42)	79.95(4)	C(6)-C(5)-H(5)	116.6(7)
C(38)-Ir(1)-C(42)	94.05(4)	C(1)-C(6)-C(5)	119.02(8)
N(2)-Ir(1)-C(43)	96.56(3)	C(1)-C(6)-C(7)	122.85(8)
O(1)-Ir(1)-C(43)	76.08(3)	C(5)-C(6)-C(7)	117.75(8)
N(1)-Ir(1)-C(43)	159.65(3)	N(1)-C(7)-C(8)	119.95(8)
O(2)-Ir(1)-C(43)	110.60(3)	N(1)-C(7)-C(6)	123.14(8)
C(39)-Ir(1)-C(43)	86.38(4)	C(8)-C(7)-C(6)	116.76(8)
C(38)-Ir(1)-C(43)	78.90(4)	C(9)-C(8)-C(7)	122.40(8)
C(42)-Ir(1)-C(43)	35.32(4)	C(9)-C(8)-H(8)	120.0(7)
C(1)-O(1)-Ir(1)	123.41(5)	C(7)-C(8)-H(8)	117.6(7)
C(17)-O(2)-Ir(1)	119.18(6)	C(10)-C(9)-C(8)	115.78(8)
C(11)-N(1)-C(7)	118.62(8)	C(10)-C(9)-C(26)	121.04(8)
C(11)-N(1)-Ir(1)	120.15(6)	C(8)-C(9)-C(26)	123.17(8)
C(7)-N(1)-Ir(1)	121.16(6)	C(9)-C(10)-C(11)	121.76(8)
C(46)-N(2)-Ir(1)	173.51(8)	C(9)-C(10)-H(10)	122.5(7)
O(1)-C(1)-C(6)	121.68(8)	C(11)-C(10)-H(10)	115.7(7)
O(1)-C(1)-C(2)	119.53(8)	N(1)-C(11)-C(10)	120.47(8)
C(6)-C(1)-C(2)	118.78(8)	N(1)-C(11)-C(12)	122.68(8)
C(3)-C(2)-C(1)	117.82(8)	C(10)-C(11)-C(12)	116.84(8)
C(3)-C(2)-C(18)	120.48(8)	C(17)-C(12)-C(13)	120.18(8)
C(1)-C(2)-C(18)	121.70(8)	C(17)-C(12)-C(11)	123.62(8)
C(4)-C(3)-C(2)	123.72(9)	C(13)-C(12)-C(11)	115.98(8)
C(4)-C(3)-H(3)	117.2(8)	C(14)-C(13)-C(12)	122.05(9)
C(2)-C(3)-H(3)	119.1(8)	C(14)-C(13)-H(13)	118.9(6)
C(5)-C(4)-C(3)	116.69(8)	C(12)-C(13)-H(13)	119.0(6)
C(5)-C(4)-C(22)	119.44(8)	C(13)-C(14)-C(15)	116.67(8)
C(3)-C(4)-C(22)	123.80(9)	C(13)-C(14)-C(30)	119.77(9)
C(4)-C(5)-C(6)	122.50(8)	C(15)-C(14)-C(30)	123.54(8)
C(4)-C(5)-H(5)	120.8(7)	C(16)-C(15)-C(14)	123.81(9)

C(16)-C(15)-H(15)	117.5(7)	C(18)-C(21)-H(21C)	108.9(9)
C(14)-C(15)-H(15)	118.6(7)	H(21A)-C(21)-H(21C)	109.2(11)
C(15)-C(16)-C(17)	117.99(9)	H(21B)-C(21)-H(21C)	111.7(11)
C(15)-C(16)-C(34)	120.23(8)	C(25)-C(22)-C(23)	109.59(12)
C(17)-C(16)-C(34)	121.76(8)	C(25)-C(22)-C(4)	112.72(9)
O(2)-C(17)-C(12)	121.23(8)	C(23)-C(22)-C(4)	109.34(9)
O(2)-C(17)-C(16)	120.13(8)	C(25)-C(22)-C(24)	107.64(10)
C(12)-C(17)-C(16)	118.53(8)	C(23)-C(22)-C(24)	108.67(12)
C(21)-C(18)-C(19)	109.52(9)	C(4)-C(22)-C(24)	108.78(10)
C(21)-C(18)-C(20)	107.35(9)	C(22)-C(23)-H(23A)	97.7(10)
C(19)-C(18)-C(20)	107.54(8)	C(22)-C(23)-H(23B)	112.4(10)
C(21)-C(18)-C(2)	110.96(8)	H(23A)-C(23)-H(23B)	122.4(13)
C(19)-C(18)-C(2)	109.66(8)	C(22)-C(23)-H(23C)	105.4(9)
C(20)-C(18)-C(2)	111.71(8)	H(23A)-C(23)-H(23C)	112.5(13)
C(18)-C(19)-H(19A)	113.2(8)	H(23B)-C(23)-H(23C)	105.2(12)
C(18)-C(19)-H(19B)	112.8(7)	C(22)-C(24)-H(24A)	111.3(12)
H(19A)-C(19)-H(19B)	106.1(11)	C(22)-C(24)-H(24B)	111.3(8)
C(18)-C(19)-H(19C)	109.6(8)	H(24A)-C(24)-H(24B)	110.9(13)
H(19A)-C(19)-H(19C)	105.4(11)	C(22)-C(24)-H(24C)	109.3(9)
H(19B)-C(19)-H(19C)	109.4(11)	H(24A)-C(24)-H(24C)	105.9(14)
C(18)-C(20)-H(20A)	109.1(8)	H(24B)-C(24)-H(24C)	108.0(13)
C(18)-C(20)-H(20B)	112.6(7)	C(22)-C(25)-H(25A)	111.2(8)
H(20A)-C(20)-H(20B)	106.3(11)	C(22)-C(25)-H(25B)	106.4(9)
C(18)-C(20)-H(20C)	112.3(8)	H(25A)-C(25)-H(25B)	109.1(12)
H(20A)-C(20)-H(20C)	105.8(11)	C(22)-C(25)-H(25C)	105.0(10)
H(20B)-C(20)-H(20C)	110.4(10)	H(25A)-C(25)-H(25C)	107.1(13)
C(18)-C(21)-H(21A)	112.4(9)	H(25B)-C(25)-H(25C)	118.0(13)
C(18)-C(21)-H(21B)	111.0(8)	C(9)-C(26)-C(29)	112.51(8)
H(21A)-C(21)-H(21B)	103.5(12)	C(9)-C(26)-C(27)	109.22(7)

C(29)-C(26)-C(27)	108.40(9)	C(30)-C(31)-H(31B)	112.9(8)
C(9)-C(26)-C(28)	108.46(8)	H(31A)-C(31)-H(31B)	107.7(13)
C(29)-C(26)-C(28)	108.45(9)	C(30)-C(31)-H(31C)	109.3(10)
C(27)-C(26)-C(28)	109.77(9)	H(31A)-C(31)-H(31C)	106.6(12)
C(26)-C(27)-H(27A)	113.4(9)	H(31B)-C(31)-H(31C)	109.0(12)
C(26)-C(27)-H(27B)	112.4(7)	C(30)-C(32)-H(32A)	110.5(8)
H(27A)-C(27)-H(27B)	102.9(12)	C(30)-C(32)-H(32B)	106.1(9)
C(26)-C(27)-H(27C)	111.4(9)	H(32A)-C(32)-H(32B)	110.5(11)
H(27A)-C(27)-H(27C)	108.9(11)	C(30)-C(32)-H(32C)	112.7(8)
H(27B)-C(27)-H(27C)	107.3(12)	H(32A)-C(32)-H(32C)	106.8(12)
C(26)-C(28)-H(28A)	106.0(8)	H(32B)-C(32)-H(32C)	110.3(11)
C(26)-C(28)-H(28B)	108.3(9)	C(30)-C(33)-H(33A)	110.1(8)
H(28A)-C(28)-H(28B)	112.2(11)	C(30)-C(33)-H(33B)	111.6(8)
C(26)-C(28)-H(28C)	108.1(8)	H(33A)-C(33)-H(33B)	107.5(10)
H(28A)-C(28)-H(28C)	109.8(13)	C(30)-C(33)-H(33C)	112.4(8)
H(28B)-C(28)-H(28C)	112.2(12)	H(33A)-C(33)-H(33C)	111.9(11)
C(26)-C(29)-H(29A)	111.7(9)	H(33B)-C(33)-H(33C)	103.0(12)
C(26)-C(29)-H(29B)	111.0(8)	C(16)-C(34)-C(37)	112.95(8)
H(29A)-C(29)-H(29B)	106.3(12)	C(16)-C(34)-C(36)	109.50(7)
C(26)-C(29)-H(29C)	111.5(10)	C(37)-C(34)-C(36)	106.34(8)
H(29A)-C(29)-H(29C)	107.8(12)	C(16)-C(34)-C(35)	109.82(8)
H(29B)-C(29)-H(29C)	108.4(11)	C(37)-C(34)-C(35)	106.58(8)
C(32)-C(30)-C(14)	112.41(9)	C(36)-C(34)-C(35)	111.60(8)
C(32)-C(30)-C(33)	108.02(8)	C(34)-C(35)-H(35A)	110.5(8)
C(14)-C(30)-C(33)	109.35(7)	C(34)-C(35)-H(35B)	110.8(8)
C(32)-C(30)-C(31)	108.67(9)	H(35A)-C(35)-H(35B)	108.6(11)
C(14)-C(30)-C(31)	109.23(8)	C(34)-C(35)-H(35C)	109.9(7)
C(33)-C(30)-C(31)	109.10(10)	H(35A)-C(35)-H(35C)	109.3(11)
C(30)-C(31)-H(31A)	111.2(9)	H(35B)-C(35)-H(35C)	107.7(10)

C(34)-C(36)-H(36A)	108.2(7)	H(40A)-C(40)-H(40B)	105.3(10)
C(34)-C(36)-H(36B)	108.8(7)	C(42)-C(41)-C(40)	114.30(9)
H(36A)-C(36)-H(36B)	108.1(11)	C(42)-C(41)-H(41A)	106.3(7)
C(34)-C(36)-H(36C)	112.2(7)	C(40)-C(41)-H(41A)	110.8(7)
H(36A)-C(36)-H(36C)	108.0(10)	C(42)-C(41)-H(41B)	107.5(7)
H(36B)-C(36)-H(36C)	111.4(10)	C(40)-C(41)-H(41B)	109.4(7)
C(34)-C(37)-H(37A)	113.1(8)	H(41A)-C(41)-H(41B)	108.3(10)
C(34)-C(37)-H(37B)	106.1(8)	C(43)-C(42)-C(41)	123.00(9)
H(37A)-C(37)-H(37B)	107.7(10)	C(43)-C(42)-Ir(1)	72.53(6)
C(34)-C(37)-H(37C)	112.0(7)	C(41)-C(42)-Ir(1)	110.15(6)
H(37A)-C(37)-H(37C)	109.5(10)	C(43)-C(42)-H(42)	116.1(7)
H(37B)-C(37)-H(37C)	108.3(10)	C(41)-C(42)-H(42)	118.6(8)
C(39)-C(38)-C(45)	125.84(9)	Ir(1)-C(42)-H(42)	101.4(8)
C(39)-C(38)-Ir(1)	70.64(5)	C(42)-C(43)-C(44)	122.13(9)
C(45)-C(38)-Ir(1)	110.12(6)	C(42)-C(43)-Ir(1)	72.15(6)
C(39)-C(38)-H(38)	114.6(7)	C(44)-C(43)-Ir(1)	112.07(6)
C(45)-C(38)-H(38)	116.0(7)	C(42)-C(43)-H(43)	116.5(7)
Ir(1)-C(38)-H(38)	107.6(7)	C(44)-C(43)-H(43)	119.4(7)
C(38)-C(39)-C(40)	125.84(9)	Ir(1)-C(43)-H(43)	98.5(7)
C(38)-C(39)-Ir(1)	72.94(5)	C(43)-C(44)-C(45)	113.40(8)
C(40)-C(39)-Ir(1)	113.00(6)	C(43)-C(44)-H(44A)	108.7(7)
C(38)-C(39)-H(39)	115.5(7)	C(45)-C(44)-H(44A)	109.7(7)
C(40)-C(39)-H(39)	115.4(7)	C(43)-C(44)-H(44B)	107.6(7)
Ir(1)-C(39)-H(39)	101.6(7)	C(45)-C(44)-H(44B)	111.1(8)
C(39)-C(40)-C(41)	115.94(8)	H(44A)-C(44)-H(44B)	106.1(11)
C(39)-C(40)-H(40A)	106.6(8)	C(38)-C(45)-C(44)	113.09(8)
C(41)-C(40)-H(40A)	111.3(7)	C(38)-C(45)-H(45A)	109.2(7)
C(39)-C(40)-H(40B)	108.6(8)	C(44)-C(45)-H(45A)	109.1(7)
C(41)-C(40)-H(40B)	108.6(7)	C(38)-C(45)-H(45B)	107.5(7)

C(44)-C(45)-H(45B)	110.5(8)	C(53)-C(52)-H(52)	119.1(8)
H(45A)-C(45)-H(45B)	107.4(10)	C(54)-C(53)-C(52)	119.35(12)
N(2)-C(46)-C(47)	177.43(12)	C(54)-C(53)-H(53)	124.3(9)
C(46)-C(47)-H(47A)	110.7(10)	C(52)-C(53)-H(53)	116.3(9)
C(46)-C(47)-H(47B)	110.4(15)	C(53)-C(54)-C(55)	120.61(11)
H(47A)-C(47)-H(47B)	120.0(18)	C(53)-C(54)-H(54)	120.4(8)
C(46)-C(47)-H(47C)	105.8(13)	C(55)-C(54)-H(54)	118.9(8)
H(47A)-C(47)-H(47C)	97.5(17)	C(54)-C(55)-C(56)	120.00(12)
H(47B)-C(47)-H(47C)	110.9(19)	C(54)-C(55)-H(55)	118.3(8)
F(4)-P(1)-F(5)	90.56(5)	C(56)-C(55)-H(55)	121.7(8)
F(4)-P(1)-F(1)	89.57(4)	C(55)-C(56)-C(51)	119.77(12)
F(5)-P(1)-F(1)	89.72(4)	C(55)-C(56)-H(56)	120.5(8)
F(4)-P(1)-F(3)	179.16(5)	C(51)-C(56)-H(56)	119.7(8)
F(5)-P(1)-F(3)	89.92(4)		
F(1)-P(1)-F(3)	89.74(4)		
F(4)-P(1)-F(6)	91.04(4)		
F(5)-P(1)-F(6)	90.36(5)		
F(1)-P(1)-F(6)	179.38(4)		
F(3)-P(1)-F(6)	89.64(4)		
F(4)-P(1)-F(2)	90.32(5)		
F(5)-P(1)-F(2)	178.92(5)		
F(1)-P(1)-F(2)	89.67(4)		
F(3)-P(1)-F(2)	89.19(4)		
F(6)-P(1)-F(2)	90.24(5)		
C(52)-C(51)-C(56)	120.40(11)		
C(52)-C(51)-H(51)	120.1(9)		
C(56)-C(51)-H(51)	119.4(9)		
C(51)-C(52)-C(53)	119.87(13)		
C(51)-C(52)-H(52)	121.1(8)		

Table S13. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	100(1)	85(1)	115(1)	30(1)	24(1)	10(1)
O(1)	115(3)	148(3)	115(3)	29(2)	21(2)	-5(2)
O(2)	171(3)	116(3)	115(3)	38(2)	33(2)	32(2)
N(1)	107(3)	103(3)	113(3)	25(3)	27(2)	16(2)
N(2)	135(3)	133(3)	130(4)	46(3)	34(3)	-5(3)
C(1)	119(4)	115(4)	135(4)	29(3)	34(3)	26(3)
C(2)	138(4)	129(4)	133(4)	13(3)	19(3)	19(3)
C(3)	184(4)	157(4)	124(4)	-2(4)	34(3)	29(3)
C(4)	153(4)	165(4)	162(4)	18(4)	65(3)	33(3)
C(5)	134(4)	142(4)	161(4)	14(3)	51(3)	8(3)
C(6)	128(4)	113(4)	123(4)	21(3)	34(3)	11(3)
C(7)	109(3)	116(4)	114(4)	24(3)	29(3)	15(3)
C(8)	136(4)	128(4)	130(4)	26(3)	50(3)	6(3)
C(9)	105(3)	109(4)	132(4)	39(3)	23(3)	14(3)
C(10)	137(4)	105(4)	109(4)	20(3)	22(3)	16(3)
C(11)	112(3)	101(4)	107(4)	34(3)	20(3)	19(3)
C(12)	114(4)	118(4)	108(4)	23(3)	27(3)	15(3)
C(13)	141(4)	115(4)	132(4)	40(3)	34(3)	14(3)
C(14)	120(4)	131(4)	137(4)	18(3)	31(3)	18(3)
C(15)	130(4)	158(4)	129(4)	31(3)	46(3)	14(3)
C(16)	107(4)	149(4)	119(4)	45(3)	25(3)	8(3)
C(17)	101(3)	121(4)	116(4)	33(3)	10(3)	12(3)
C(18)	150(4)	166(4)	146(4)	3(4)	5(3)	7(3)
C(19)	161(4)	263(6)	204(5)	5(4)	-4(4)	45(4)

C(20)	209(5)	276(6)	154(5)	-9(4)	-3(4)	1(4)
C(21)	229(5)	185(5)	219(5)	26(4)	-14(4)	-50(4)
C(22)	207(5)	263(5)	211(5)	-27(4)	120(4)	13(4)
C(23)	584(9)	381(8)	449(9)	21(7)	366(8)	-67(7)
C(24)	220(6)	680(11)	328(7)	-65(7)	86(5)	135(6)
C(25)	279(6)	441(8)	233(6)	-54(6)	131(5)	25(5)
C(26)	141(4)	104(4)	158(4)	27(3)	47(3)	-4(3)
C(27)	249(5)	134(4)	362(6)	99(4)	130(5)	41(4)
C(28)	185(5)	214(5)	284(6)	64(5)	-22(4)	-39(4)
C(29)	286(5)	215(5)	209(5)	24(4)	114(4)	-86(4)
C(30)	165(4)	136(4)	170(4)	23(4)	48(3)	38(3)
C(31)	301(6)	273(6)	281(6)	13(5)	-19(5)	155(5)
C(32)	278(5)	162(5)	269(6)	3(4)	154(4)	31(4)
C(33)	250(5)	135(4)	256(5)	36(4)	99(4)	16(4)
C(34)	140(4)	165(4)	134(4)	62(3)	36(3)	11(3)
C(35)	165(4)	196(5)	205(5)	81(4)	35(4)	-12(3)
C(36)	171(4)	224(5)	163(4)	99(4)	20(3)	34(4)
C(37)	227(5)	245(5)	167(5)	89(4)	83(4)	35(4)
C(38)	118(4)	137(4)	188(4)	50(4)	28(3)	48(3)
C(39)	131(4)	148(4)	179(4)	43(4)	7(3)	51(3)
C(40)	227(5)	170(4)	195(5)	76(4)	24(4)	75(4)
C(41)	257(5)	138(4)	194(5)	81(4)	50(4)	31(3)
C(42)	168(4)	118(4)	203(5)	64(4)	46(3)	-5(3)
C(43)	168(4)	106(4)	201(5)	49(4)	30(3)	-19(3)
C(44)	232(5)	108(4)	196(5)	28(4)	36(4)	21(3)
C(45)	203(4)	124(4)	185(5)	33(4)	44(4)	54(3)
C(46)	154(4)	168(4)	186(4)	80(4)	60(3)	15(3)
C(47)	231(5)	294(6)	533(9)	242(6)	207(5)	147(5)

P(1)	165(1)	214(1)	270(1)	34(1)	54(1)	-27(1)
F(1)	216(3)	254(3)	311(4)	55(3)	1(3)	-56(2)
F(2)	311(4)	378(4)	444(5)	247(4)	-5(3)	-17(3)
F(3)	208(3)	309(4)	342(4)	123(3)	95(3)	-4(2)
F(4)	300(4)	646(6)	370(4)	-3(4)	179(3)	-87(4)
F(5)	304(4)	237(4)	733(6)	104(4)	58(4)	72(3)
F(6)	298(4)	427(5)	370(4)	-84(4)	30(3)	-110(3)
C(51)	200(5)	445(7)	320(6)	242(6)	37(4)	23(5)
C(52)	342(6)	309(6)	301(6)	134(5)	65(5)	-62(5)
C(53)	316(6)	311(6)	406(7)	173(6)	120(5)	110(5)
C(54)	235(5)	429(7)	304(6)	150(6)	35(5)	104(5)
C(55)	294(6)	366(7)	237(6)	79(5)	75(4)	55(5)
C(56)	270(5)	373(7)	293(6)	189(5)	136(5)	132(5)

Table S14. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6**.

	x	y	z	U_{iso}
H(3)	5889(10)	7964(11)	10260(7)	20(3)
H(5)	3669(10)	5717(10)	8689(6)	14(3)
H(8)	4134(10)	4116(10)	8239(6)	15(3)
H(10)	4832(10)	2568(11)	6344(6)	15(3)
H(13)	6763(9)	2350(10)	6258(6)	8(3)
H(15)	8013(9)	3269(10)	4700(6)	12(3)
H(19A)	9039(11)	7311(12)	9149(7)	25(3)
H(19B)	8859(10)	6867(12)	9769(7)	24(3)
H(19C)	9766(11)	8029(12)	9834(7)	27(3)
H(20A)	8865(11)	9246(12)	10724(7)	28(3)
H(20B)	7909(11)	8194(12)	10763(7)	24(3)
H(20C)	7487(10)	9411(11)	10660(6)	20(3)
H(21A)	8909(13)	9948(14)	9706(8)	43(4)
H(21B)	7497(12)	9922(13)	9537(7)	32(4)
H(21C)	8228(11)	9142(12)	9003(7)	24(3)
H(23A)	4041(16)	5632(16)	10391(10)	66(5)
H(23B)	2934(14)	5019(16)	9564(9)	58(5)
H(23C)	2438(14)	5687(14)	10286(8)	50(4)
H(24A)	1749(16)	7309(16)	9852(10)	67(6)
H(24B)	2133(12)	6691(14)	9139(8)	39(4)
H(24C)	2614(13)	8080(16)	9528(8)	46(5)
H(25A)	3123(12)	7793(13)	10939(7)	33(4)
H(25B)	4042(12)	8562(14)	10614(8)	37(4)
H(25C)	4478(15)	7465(16)	10933(9)	61(5)
H(27A)	4264(12)	821(13)	6600(8)	38(4)

H(27B)	3490(11)	244(12)	7001(7)	25(3)
H(27C)	4707(12)	993(13)	7372(8)	35(4)
H(28A)	1906(12)	2692(14)	6823(7)	37(4)
H(28B)	1672(13)	1261(14)	6662(8)	43(4)
H(28C)	2551(12)	1915(12)	6261(8)	33(4)
H(29A)	3544(12)	2161(13)	8275(8)	37(4)
H(29B)	2382(11)	1432(12)	7880(7)	26(3)
H(29C)	2458(12)	2756(14)	8048(8)	40(4)
H(31A)	9096(13)	440(14)	5690(8)	44(4)
H(31B)	8527(11)	1324(12)	6251(8)	31(4)
H(31C)	9568(13)	1757(14)	5873(8)	41(4)
H(32A)	7927(11)	1263(12)	4209(7)	25(3)
H(32B)	8711(11)	395(13)	4481(7)	33(4)
H(32C)	9223(12)	1761(13)	4625(7)	33(4)
H(33A)	6156(11)	554(12)	4737(7)	24(3)
H(33B)	6408(11)	486(12)	5501(7)	24(3)
H(33C)	6987(11)	-324(13)	4985(7)	29(3)
H(35A)	8479(11)	6794(12)	5725(7)	26(3)
H(35B)	8646(11)	7120(13)	5051(7)	30(4)
H(35C)	9410(11)	6174(11)	5284(6)	24(3)
H(36A)	5782(10)	5331(11)	4450(6)	17(3)
H(36B)	6493(10)	6519(12)	4489(7)	22(3)
H(36C)	6007(10)	6309(11)	5156(6)	19(3)
H(37A)	8756(11)	4664(11)	4239(6)	23(3)
H(37B)	7980(11)	5513(12)	3954(7)	25(3)
H(37C)	7355(10)	4234(11)	3921(6)	19(3)
H(38)	4632(10)	7189(10)	7659(6)	14(3)
H(39)	4672(9)	6653(10)	6549(6)	13(3)
H(40A)	5167(10)	8944(11)	6575(6)	20(3)

H(40B)	5045(10)	7906(11)	5923(6)	18(3)
H(41A)	7053(10)	8004(11)	5913(6)	18(3)
H(41B)	7083(10)	9284(11)	6360(6)	17(3)
H(42)	8459(10)	7883(11)	6779(6)	19(3)
H(43)	8349(9)	8572(10)	7879(6)	12(3)
H(44A)	6579(10)	9911(11)	7490(6)	17(3)
H(44B)	7222(10)	10087(12)	8232(7)	23(3)
H(45A)	5761(9)	8829(10)	8445(6)	12(3)
H(45B)	4945(11)	9375(12)	7966(7)	26(3)
H(47A)	10148(14)	4244(16)	7438(9)	55(5)
H(47B)	10970(20)	5290(20)	7299(12)	108(8)
H(47C)	10080(20)	4250(20)	6733(14)	112(8)
H(51)	7134(12)	3302(13)	7720(7)	36(4)
H(52)	8172(12)	1627(14)	7516(8)	38(4)
H(53)	10025(12)	1724(13)	8141(7)	37(4)
H(54)	10960(12)	3439(12)	9021(7)	28(3)
H(55)	9942(12)	5092(13)	9216(8)	37(4)
H(56)	7988(11)	5001(12)	8562(7)	29(4)

(ONO^{tBu})Ir(cod)OTf, 7

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	8172(1)	5229(1)	8375(1)	7(1)
S(1)	6161(1)	4725(1)	7454(1)	10(1)
F(1)	5467(1)	6398(1)	6794(1)	45(1)
F(2)	4595(1)	6162(1)	8086(1)	44(1)
F(3)	4109(1)	5285(1)	7235(1)	29(1)
O(1)	8526(1)	3826(1)	7905(1)	10(1)
O(2)	7672(1)	6756(1)	8546(1)	10(1)
O(3)	7090(1)	5364(1)	7580(1)	12(1)
O(4)	5565(1)	4091(1)	8153(1)	19(1)
O(5)	6505(1)	4297(1)	6678(1)	21(1)
N(1)	9610(1)	5673(1)	7385(1)	8(1)
C(1)	9630(1)	3398(1)	7662(1)	10(1)
C(2)	9773(1)	2321(1)	7643(1)	12(1)
C(3)	10919(1)	1894(1)	7550(1)	13(1)
C(4)	11937(1)	2467(1)	7452(1)	12(1)
C(5)	11795(1)	3510(1)	7354(1)	11(1)
C(6)	10669(1)	3986(1)	7412(1)	10(1)
C(7)	10624(1)	5068(1)	7132(1)	9(1)
C(8)	11636(1)	5435(1)	6531(1)	10(1)
C(9)	11671(1)	6418(1)	6189(1)	10(1)
C(10)	10605(1)	6995(1)	6437(1)	10(1)
C(11)	9574(1)	6605(1)	6994(1)	9(1)
C(12)	8458(1)	7236(1)	7123(1)	9(1)

C(13)	8310(1)	7781(1)	6430(1)	11(1)
C(14)	7380(1)	8496(1)	6485(1)	12(1)
C(15)	6649(1)	8694(1)	7268(1)	12(1)
C(16)	6740(1)	8167(1)	7980(1)	10(1)
C(17)	7617(1)	7351(1)	7893(1)	9(1)
C(18)	8716(1)	1640(1)	7700(1)	14(1)
C(19)	8160(1)	1992(1)	7022(1)	20(1)
C(20)	7755(1)	1694(1)	8533(1)	20(1)
C(21)	9122(1)	523(1)	7579(1)	22(1)
C(22)	13150(1)	1975(1)	7462(1)	14(1)
C(23)	13351(1)	2174(1)	8277(1)	29(1)
C(24)	14183(1)	2438(1)	6769(1)	21(1)
C(25)	13198(1)	830(1)	7366(1)	25(1)
C(26)	12786(1)	6863(1)	5566(1)	11(1)
C(27)	13776(1)	6050(1)	5262(1)	18(1)
C(28)	13256(1)	7681(1)	5974(1)	18(1)
C(29)	12450(1)	7354(1)	4826(1)	16(1)
C(30)	7230(1)	9034(1)	5702(1)	16(1)
C(31)	6164(1)	9799(1)	5883(1)	26(1)
C(32)	8370(1)	9611(1)	5248(1)	27(1)
C(33)	7020(1)	8245(1)	5154(1)	27(1)
C(34)	5950(1)	8492(1)	8820(1)	12(1)
C(35)	6739(1)	8665(1)	9365(1)	15(1)
C(36)	5244(1)	9494(1)	8760(1)	16(1)
C(37)	5017(1)	7690(1)	9228(1)	15(1)
C(38)	5033(1)	5704(1)	7387(1)	22(1)
C(39)	8940(1)	5684(1)	9293(1)	11(1)
C(40)	9408(1)	4715(1)	9062(1)	11(1)
C(41)	9017(1)	3736(1)	9552(1)	13(1)

C(42)	7649(1)	3679(1)	9918(1)	14(1)
C(43)	6971(1)	4222(1)	9382(1)	12(1)
C(44)	6534(1)	5212(1)	9487(1)	12(1)
C(45)	6710(1)	5858(1)	10124(1)	14(1)
C(46)	8030(1)	5906(1)	10107(1)	15(1)
C(51)	2170(1)	8360(1)	8461(1)	25(1)
C(52)	1234(1)	8076(1)	8190(1)	25(1)
C(53)	55(1)	8204(1)	8677(1)	22(1)
C(54)	-188(1)	8599(1)	9433(1)	23(1)
C(55)	748(1)	8877(1)	9706(1)	22(1)
C(56)	1922(1)	8766(1)	9215(1)	22(1)
C(61)	10437(1)	4147(1)	5350(1)	19(1)
C(62)	9324(1)	4582(1)	5752(1)	18(1)
C(63)	8887(1)	5434(1)	5403(1)	19(1)

Table S16. Selected bond lengths [Å] and angles [°] for **7**.

Ir(1)-O(1)	2.0431(6)	O(1)-Ir(1)-N(1)	84.59(2)
Ir(1)-N(1)	2.0738(6)	O(1)-Ir(1)-O(2)	163.22(2)
Ir(1)-O(2)	2.0836(6)	N(1)-Ir(1)-O(2)	88.90(2)
Ir(1)-O(3)	2.1247(6)	O(1)-Ir(1)-O(3)	80.91(2)
Ir(1)-C(39)	2.1725(8)	N(1)-Ir(1)-O(3)	87.90(2)
Ir(1)-C(40)	2.1865(8)	O(2)-Ir(1)-O(3)	83.42(2)
Ir(1)-C(44)	2.2592(8)	O(1)-Ir(1)-C(39)	121.97(3)
Ir(1)-C(43)	2.2656(8)	N(1)-Ir(1)-C(39)	95.20(3)
		O(2)-Ir(1)-C(39)	73.96(3)
		O(3)-Ir(1)-C(39)	157.08(3)
		O(1)-Ir(1)-C(40)	84.60(3)
		N(1)-Ir(1)-C(40)	90.09(3)
		O(2)-Ir(1)-C(40)	110.91(3)
		O(3)-Ir(1)-C(40)	165.50(3)
		C(39)-Ir(1)-C(40)	37.42(3)
		O(1)-Ir(1)-C(44)	110.92(3)
		N(1)-Ir(1)-C(44)	164.19(3)
		O(2)-Ir(1)-C(44)	75.34(3)
		O(3)-Ir(1)-C(44)	91.51(3)
		C(39)-Ir(1)-C(44)	79.40(3)
		C(40)-Ir(1)-C(44)	94.28(3)
		O(1)-Ir(1)-C(43)	77.60(3)
		N(1)-Ir(1)-C(43)	159.93(3)
		O(2)-Ir(1)-C(43)	110.72(3)
		O(3)-Ir(1)-C(43)	98.24(3)
		C(39)-Ir(1)-C(43)	86.58(3)
		C(40)-Ir(1)-C(43)	79.18(3)

C(44)-Ir(1)-C(43)	35.50(3)

Table S17. Bond lengths [Å] and angles [°] for **7**.

Ir(1)-O(1)	2.0431(6)	C(3)-H(3)	0.931(12)
Ir(1)-N(1)	2.0738(6)	C(4)-C(5)	1.3818(11)
Ir(1)-O(2)	2.0836(6)	C(4)-C(22)	1.5360(11)
Ir(1)-O(3)	2.1247(6)	C(5)-C(6)	1.4093(11)
Ir(1)-C(39)	2.1725(8)	C(5)-H(5)	0.958(10)
Ir(1)-C(40)	2.1865(8)	C(6)-C(7)	1.4779(10)
Ir(1)-C(44)	2.2592(8)	C(7)-C(8)	1.3978(11)
Ir(1)-C(43)	2.2656(8)	C(8)-C(9)	1.3845(11)
S(1)-O(5)	1.4211(8)	C(8)-H(8)	0.948(11)
S(1)-O(4)	1.4302(7)	C(9)-C(10)	1.3926(11)
S(1)-O(3)	1.4836(6)	C(9)-C(26)	1.5289(11)
S(1)-C(38)	1.8223(9)	C(10)-C(11)	1.3907(11)
F(1)-C(38)	1.3192(13)	C(10)-H(10)	0.955(11)
F(2)-C(38)	1.3296(14)	C(11)-C(12)	1.4782(10)
F(3)-C(38)	1.3407(11)	C(12)-C(13)	1.4009(11)
O(1)-C(1)	1.3387(9)	C(12)-C(17)	1.4020(11)
O(2)-C(17)	1.3421(9)	C(13)-C(14)	1.3882(11)
N(1)-C(11)	1.3656(10)	C(13)-H(13)	0.969(12)
N(1)-C(7)	1.3682(10)	C(14)-C(15)	1.3937(13)
C(1)-C(6)	1.4136(11)	C(14)-C(30)	1.5331(12)
C(1)-C(2)	1.4232(11)	C(15)-C(16)	1.3964(12)
C(2)-C(3)	1.3946(11)	C(15)-H(15)	0.956(12)
C(2)-C(18)	1.5422(11)	C(16)-C(17)	1.4313(10)
C(3)-C(4)	1.4046(12)	C(16)-C(34)	1.5355(12)

C(18)-C(20)	1.5328(14)	C(27)-H(27C)	0.938(14)
C(18)-C(21)	1.5335(13)	C(28)-H(28A)	0.974(13)
C(18)-C(19)	1.5360(13)	C(28)-H(28B)	0.985(13)
C(19)-H(19A)	0.967(14)	C(28)-H(28C)	0.959(14)
C(19)-H(19B)	0.952(15)	C(29)-H(29A)	0.933(15)
C(19)-H(19C)	0.927(14)	C(29)-H(29B)	0.969(12)
C(20)-H(20A)	0.974(14)	C(29)-H(29C)	0.999(13)
C(20)-H(20B)	0.950(14)	C(30)-C(33)	1.5290(16)
C(20)-H(20C)	0.955(15)	C(30)-C(31)	1.5330(13)
C(21)-H(21A)	0.988(14)	C(30)-C(32)	1.5352(14)
C(21)-H(21B)	0.966(15)	C(31)-H(31A)	0.947(14)
C(21)-H(21C)	0.988(13)	C(31)-H(31B)	0.977(16)
C(22)-C(25)	1.5269(13)	C(31)-H(31C)	0.974(16)
C(22)-C(23)	1.5332(15)	C(32)-H(32A)	0.983(18)
C(22)-C(24)	1.5352(13)	C(32)-H(32B)	0.955(17)
C(23)-H(23A)	0.946(14)	C(32)-H(32C)	0.974(15)
C(23)-H(23B)	1.026(16)	C(33)-H(33A)	0.957(15)
C(23)-H(23C)	0.998(15)	C(33)-H(33B)	0.961(17)
C(24)-H(24A)	0.953(14)	C(33)-H(33C)	0.972(15)
C(24)-H(24B)	0.962(14)	C(34)-C(37)	1.5345(12)
C(24)-H(24C)	1.008(17)	C(34)-C(36)	1.5358(11)
C(25)-H(25A)	1.000(13)	C(34)-C(35)	1.5396(12)
C(25)-H(25B)	0.939(16)	C(35)-H(35A)	0.988(12)
C(25)-H(25C)	0.969(14)	C(35)-H(35B)	0.963(15)
C(26)-C(27)	1.5327(12)	C(35)-H(35C)	0.974(13)
C(26)-C(28)	1.5363(13)	C(36)-H(36A)	0.987(13)
C(26)-C(29)	1.5369(12)	C(36)-H(36B)	0.980(15)
C(27)-H(27A)	0.997(12)	C(36)-H(36C)	0.977(13)
C(27)-H(27B)	0.982(12)	C(37)-H(37A)	0.976(13)

C(37)-H(37B)	0.991(14)	C(54)-C(55)	1.3909(15)
C(37)-H(37C)	0.951(12)	C(54)-H(54)	0.965(14)
C(39)-C(40)	1.3985(12)	C(55)-C(56)	1.3842(15)
C(39)-C(46)	1.5158(12)	C(55)-H(55)	0.931(16)
C(39)-H(39)	0.958(11)	C(56)-H(56)	0.940(14)
C(40)-C(41)	1.5056(11)	C(61)-C(63)#1	1.3899(14)
C(40)-H(40)	0.975(10)	C(61)-C(62)	1.3906(14)
C(41)-C(42)	1.5362(12)	C(61)-H(61)	0.960(13)
C(41)-H(41A)	0.958(12)	C(62)-C(63)	1.3867(14)
C(41)-H(41B)	0.945(12)	C(62)-H(62)	0.926(13)
C(42)-C(43)	1.5142(12)	C(63)-C(61)#1	1.3899(14)
C(42)-H(42A)	0.975(12)	C(63)-H(63)	0.963(13)
C(42)-H(42B)	0.974(13)		
C(43)-C(44)	1.3795(12)	O(1)-Ir(1)-N(1)	84.59(2)
C(43)-H(43)	0.931(12)	O(1)-Ir(1)-O(2)	163.22(2)
C(44)-C(45)	1.5017(13)	N(1)-Ir(1)-O(2)	88.90(2)
C(44)-H(44)	0.967(12)	O(1)-Ir(1)-O(3)	80.91(2)
C(45)-C(46)	1.5411(12)	N(1)-Ir(1)-O(3)	87.90(2)
C(45)-H(45A)	0.956(13)	O(2)-Ir(1)-O(3)	83.42(2)
C(45)-H(45B)	0.908(11)	O(1)-Ir(1)-C(39)	121.97(3)
C(46)-H(46A)	0.944(13)	N(1)-Ir(1)-C(39)	95.20(3)
C(46)-H(46B)	0.978(12)	O(2)-Ir(1)-C(39)	73.96(3)
C(51)-C(56)	1.3799(17)	O(3)-Ir(1)-C(39)	157.08(3)
C(51)-C(52)	1.3908(15)	O(1)-Ir(1)-C(40)	84.60(3)
C(51)-H(51)	0.974(15)	N(1)-Ir(1)-C(40)	90.09(3)
C(52)-C(53)	1.3884(16)	O(2)-Ir(1)-C(40)	110.91(3)
C(52)-H(52)	0.940(17)	O(3)-Ir(1)-C(40)	165.50(3)
C(53)-C(54)	1.3785(17)	C(39)-Ir(1)-C(40)	37.42(3)
C(53)-H(53)	0.931(14)	O(1)-Ir(1)-C(44)	110.92(3)

N(1)-Ir(1)-C(44)	164.19(3)	C(1)-C(2)-C(18)	121.84(7)
O(2)-Ir(1)-C(44)	75.34(3)	C(2)-C(3)-C(4)	123.78(7)
O(3)-Ir(1)-C(44)	91.51(3)	C(2)-C(3)-H(3)	119.1(7)
C(39)-Ir(1)-C(44)	79.40(3)	C(4)-C(3)-H(3)	117.1(7)
C(40)-Ir(1)-C(44)	94.28(3)	C(5)-C(4)-C(3)	116.66(7)
O(1)-Ir(1)-C(43)	77.60(3)	C(5)-C(4)-C(22)	120.85(7)
N(1)-Ir(1)-C(43)	159.93(3)	C(3)-C(4)-C(22)	122.48(7)
O(2)-Ir(1)-C(43)	110.72(3)	C(4)-C(5)-C(6)	121.96(7)
O(3)-Ir(1)-C(43)	98.24(3)	C(4)-C(5)-H(5)	120.0(6)
C(39)-Ir(1)-C(43)	86.58(3)	C(6)-C(5)-H(5)	118.0(6)
C(40)-Ir(1)-C(43)	79.18(3)	C(5)-C(6)-C(1)	119.39(7)
C(44)-Ir(1)-C(43)	35.50(3)	C(5)-C(6)-C(7)	118.66(7)
O(5)-S(1)-O(4)	117.88(5)	C(1)-C(6)-C(7)	121.68(7)
O(5)-S(1)-O(3)	113.56(4)	N(1)-C(7)-C(8)	120.26(7)
O(4)-S(1)-O(3)	114.24(4)	N(1)-C(7)-C(6)	122.44(7)
O(5)-S(1)-C(38)	104.14(5)	C(8)-C(7)-C(6)	117.04(7)
O(4)-S(1)-C(38)	104.07(5)	C(9)-C(8)-C(7)	122.10(7)
O(3)-S(1)-C(38)	100.07(4)	C(9)-C(8)-H(8)	119.9(7)
C(1)-O(1)-Ir(1)	123.10(5)	C(7)-C(8)-H(8)	117.9(7)
C(17)-O(2)-Ir(1)	118.01(5)	C(8)-C(9)-C(10)	115.80(7)
S(1)-O(3)-Ir(1)	133.82(4)	C(8)-C(9)-C(26)	123.44(7)
C(11)-N(1)-C(7)	118.74(6)	C(10)-C(9)-C(26)	120.75(7)
C(11)-N(1)-Ir(1)	119.81(5)	C(11)-C(10)-C(9)	121.94(7)
C(7)-N(1)-Ir(1)	121.39(5)	C(11)-C(10)-H(10)	115.4(7)
O(1)-C(1)-C(6)	122.00(7)	C(9)-C(10)-H(10)	122.7(7)
O(1)-C(1)-C(2)	119.54(7)	N(1)-C(11)-C(10)	120.44(7)
C(6)-C(1)-C(2)	118.46(7)	N(1)-C(11)-C(12)	122.67(7)
C(3)-C(2)-C(1)	117.69(7)	C(10)-C(11)-C(12)	116.88(6)
C(3)-C(2)-C(18)	120.45(7)	C(13)-C(12)-C(17)	120.52(7)

C(13)-C(12)-C(11)	116.03(7)	C(18)-C(20)-H(20A)	109.6(9)
C(17)-C(12)-C(11)	123.32(7)	C(18)-C(20)-H(20B)	109.7(8)
C(14)-C(13)-C(12)	121.72(8)	H(20A)-C(20)-H(20B)	108.5(11)
C(14)-C(13)-H(13)	119.2(7)	C(18)-C(20)-H(20C)	111.0(8)
C(12)-C(13)-H(13)	119.1(7)	H(20A)-C(20)-H(20C)	109.3(12)
C(13)-C(14)-C(15)	116.60(7)	H(20B)-C(20)-H(20C)	108.7(12)
C(13)-C(14)-C(30)	119.42(8)	C(18)-C(21)-H(21A)	111.6(8)
C(15)-C(14)-C(30)	123.97(7)	C(18)-C(21)-H(21B)	110.5(8)
C(14)-C(15)-C(16)	124.20(7)	H(21A)-C(21)-H(21B)	110.9(11)
C(14)-C(15)-H(15)	118.1(8)	C(18)-C(21)-H(21C)	110.1(8)
C(16)-C(15)-H(15)	117.7(8)	H(21A)-C(21)-H(21C)	105.4(11)
C(15)-C(16)-C(17)	117.54(7)	H(21B)-C(21)-H(21C)	108.0(12)
C(15)-C(16)-C(34)	120.21(7)	C(25)-C(22)-C(23)	109.17(9)
C(17)-C(16)-C(34)	122.21(7)	C(25)-C(22)-C(24)	107.78(8)
O(2)-C(17)-C(12)	121.26(7)	C(23)-C(22)-C(24)	108.22(9)
O(2)-C(17)-C(16)	120.31(7)	C(25)-C(22)-C(4)	111.97(8)
C(12)-C(17)-C(16)	118.30(7)	C(23)-C(22)-C(4)	108.51(8)
C(20)-C(18)-C(21)	107.82(8)	C(24)-C(22)-C(4)	111.11(7)
C(20)-C(18)-C(19)	109.42(8)	C(22)-C(23)-H(23A)	106.0(9)
C(21)-C(18)-C(19)	107.42(8)	C(22)-C(23)-H(23B)	111.0(9)
C(20)-C(18)-C(2)	111.23(8)	H(23A)-C(23)-H(23B)	114.4(12)
C(21)-C(18)-C(2)	111.89(7)	C(22)-C(23)-H(23C)	111.4(10)
C(19)-C(18)-C(2)	108.97(7)	H(23A)-C(23)-H(23C)	105.0(12)
C(18)-C(19)-H(19A)	110.7(9)	H(23B)-C(23)-H(23C)	109.1(12)
C(18)-C(19)-H(19B)	111.4(8)	C(22)-C(24)-H(24A)	108.2(8)
H(19A)-C(19)-H(19B)	105.9(13)	C(22)-C(24)-H(24B)	111.3(8)
C(18)-C(19)-H(19C)	112.8(9)	H(24A)-C(24)-H(24B)	106.8(11)
H(19A)-C(19)-H(19C)	107.1(11)	C(22)-C(24)-H(24C)	110.7(8)
H(19B)-C(19)-H(19C)	108.6(12)	H(24A)-C(24)-H(24C)	109.5(12)

H(24B)-C(24)-H(24C)	110.2(12)	H(29A)-C(29)-H(29C)	111.6(11)
C(22)-C(25)-H(25A)	109.8(8)	H(29B)-C(29)-H(29C)	109.9(10)
C(22)-C(25)-H(25B)	112.1(9)	C(33)-C(30)-C(31)	108.21(9)
H(25A)-C(25)-H(25B)	108.5(12)	C(33)-C(30)-C(14)	109.35(8)
C(22)-C(25)-H(25C)	112.6(9)	C(31)-C(30)-C(14)	112.01(8)
H(25A)-C(25)-H(25C)	106.7(11)	C(33)-C(30)-C(32)	109.43(9)
H(25B)-C(25)-H(25C)	106.9(12)	C(31)-C(30)-C(32)	108.23(8)
C(9)-C(26)-C(27)	112.06(7)	C(14)-C(30)-C(32)	109.57(8)
C(9)-C(26)-C(28)	108.28(7)	C(30)-C(31)-H(31A)	111.0(8)
C(27)-C(26)-C(28)	109.44(7)	C(30)-C(31)-H(31B)	110.1(9)
C(9)-C(26)-C(29)	109.55(6)	H(31A)-C(31)-H(31B)	108.4(12)
C(27)-C(26)-C(29)	108.25(8)	C(30)-C(31)-H(31C)	112.0(8)
C(28)-C(26)-C(29)	109.24(7)	H(31A)-C(31)-H(31C)	106.9(12)
C(26)-C(27)-H(27A)	110.8(7)	H(31B)-C(31)-H(31C)	108.4(12)
C(26)-C(27)-H(27B)	109.3(7)	C(30)-C(32)-H(32A)	109.0(9)
H(27A)-C(27)-H(27B)	108.3(10)	C(30)-C(32)-H(32B)	110.8(9)
C(26)-C(27)-H(27C)	113.4(8)	H(32A)-C(32)-H(32B)	107.3(13)
H(27A)-C(27)-H(27C)	109.0(11)	C(30)-C(32)-H(32C)	113.1(8)
H(27B)-C(27)-H(27C)	105.8(11)	H(32A)-C(32)-H(32C)	110.7(13)
C(26)-C(28)-H(28A)	110.8(8)	H(32B)-C(32)-H(32C)	105.7(13)
C(26)-C(28)-H(28B)	109.6(9)	C(30)-C(33)-H(33A)	112.8(9)
H(28A)-C(28)-H(28B)	108.4(11)	C(30)-C(33)-H(33B)	111.7(10)
C(26)-C(28)-H(28C)	111.0(8)	H(33A)-C(33)-H(33B)	108.0(14)
H(28A)-C(28)-H(28C)	107.0(12)	C(30)-C(33)-H(33C)	111.0(10)
H(28B)-C(28)-H(28C)	110.0(11)	H(33A)-C(33)-H(33C)	106.3(12)
C(26)-C(29)-H(29A)	109.7(8)	H(33B)-C(33)-H(33C)	106.6(12)
C(26)-C(29)-H(29B)	108.7(7)	C(37)-C(34)-C(16)	110.76(7)
H(29A)-C(29)-H(29B)	107.7(12)	C(37)-C(34)-C(36)	106.46(7)
C(26)-C(29)-H(29C)	109.2(8)	C(16)-C(34)-C(36)	112.28(7)

C(37)-C(34)-C(35)	110.49(7)	C(46)-C(39)-Ir(1)	114.56(5)
C(16)-C(34)-C(35)	109.85(6)	C(40)-C(39)-H(39)	116.3(7)
C(36)-C(34)-C(35)	106.90(7)	C(46)-C(39)-H(39)	114.8(7)
C(34)-C(35)-H(35A)	112.2(7)	Ir(1)-C(39)-H(39)	104.0(7)
C(34)-C(35)-H(35B)	110.0(8)	C(39)-C(40)-C(41)	125.29(8)
H(35A)-C(35)-H(35B)	107.8(11)	C(39)-C(40)-Ir(1)	70.75(4)
C(34)-C(35)-H(35C)	109.3(8)	C(41)-C(40)-Ir(1)	111.26(5)
H(35A)-C(35)-H(35C)	108.6(10)	C(39)-C(40)-H(40)	115.0(6)
H(35B)-C(35)-H(35C)	108.8(12)	C(41)-C(40)-H(40)	115.9(6)
C(34)-C(36)-H(36A)	112.4(7)	Ir(1)-C(40)-H(40)	106.6(6)
C(34)-C(36)-H(36B)	108.0(8)	C(40)-C(41)-C(42)	113.15(7)
H(36A)-C(36)-H(36B)	108.1(11)	C(40)-C(41)-H(41A)	108.7(7)
C(34)-C(36)-H(36C)	111.6(7)	C(42)-C(41)-H(41A)	108.9(7)
H(36A)-C(36)-H(36C)	108.7(10)	C(40)-C(41)-H(41B)	108.3(7)
H(36B)-C(36)-H(36C)	108.0(10)	C(42)-C(41)-H(41B)	110.1(7)
C(34)-C(37)-H(37A)	108.9(7)	H(41A)-C(41)-H(41B)	107.5(10)
C(34)-C(37)-H(37B)	110.6(7)	C(43)-C(42)-C(41)	113.19(7)
H(37A)-C(37)-H(37B)	108.6(10)	C(43)-C(42)-H(42A)	108.2(7)
C(34)-C(37)-H(37C)	111.5(7)	C(41)-C(42)-H(42A)	110.2(7)
H(37A)-C(37)-H(37C)	108.4(11)	C(43)-C(42)-H(42B)	108.9(7)
H(37B)-C(37)-H(37C)	108.8(10)	C(41)-C(42)-H(42B)	111.0(7)
F(1)-C(38)-F(2)	108.81(9)	H(42A)-C(42)-H(42B)	104.9(10)
F(1)-C(38)-F(3)	107.61(9)	C(44)-C(43)-C(42)	122.66(8)
F(2)-C(38)-F(3)	107.12(9)	C(44)-C(43)-Ir(1)	72.00(5)
F(1)-C(38)-S(1)	111.82(7)	C(42)-C(43)-Ir(1)	112.00(5)
F(2)-C(38)-S(1)	111.28(7)	C(44)-C(43)-H(43)	117.8(7)
F(3)-C(38)-S(1)	110.02(7)	C(42)-C(43)-H(43)	117.2(7)
C(40)-C(39)-C(46)	124.57(7)	Ir(1)-C(43)-H(43)	100.8(7)
C(40)-C(39)-Ir(1)	71.83(5)	C(43)-C(44)-C(45)	123.60(8)

C(43)-C(44)-Ir(1)	72.50(5)	C(56)-C(55)-C(54)	119.97(11)
C(45)-C(44)-Ir(1)	110.55(5)	C(56)-C(55)-H(55)	119.4(8)
C(43)-C(44)-H(44)	116.2(7)	C(54)-C(55)-H(55)	120.6(8)
C(45)-C(44)-H(44)	117.7(8)	C(51)-C(56)-C(55)	120.16(10)
Ir(1)-C(44)-H(44)	101.9(7)	C(51)-C(56)-H(56)	121.1(9)
C(44)-C(45)-C(46)	113.55(7)	C(55)-C(56)-H(56)	118.7(9)
C(44)-C(45)-H(45A)	108.3(8)	C(63)#1-C(61)-C(62)	120.09(9)
C(46)-C(45)-H(45A)	111.1(7)	C(63)#1-C(61)-H(61)	120.6(8)
C(44)-C(45)-H(45B)	110.3(8)	C(62)-C(61)-H(61)	119.3(8)
C(46)-C(45)-H(45B)	108.5(7)	C(63)-C(62)-C(61)	120.02(9)
H(45A)-C(45)-H(45B)	104.7(10)	C(63)-C(62)-H(62)	120.1(8)
C(39)-C(46)-C(45)	114.75(7)	C(61)-C(62)-H(62)	119.9(8)
C(39)-C(46)-H(46A)	108.0(8)	C(62)-C(63)-C(61)#1	119.89(9)
C(45)-C(46)-H(46A)	108.1(7)	C(62)-C(63)-H(63)	120.3(8)
C(39)-C(46)-H(46B)	107.6(7)	C(61)#1-C(63)-H(63)	119.8(8)
C(45)-C(46)-H(46B)	111.8(7)		
H(46A)-C(46)-H(46B)	106.2(11)		
C(56)-C(51)-C(52)	119.85(10)		
C(56)-C(51)-H(51)	122.4(9)		
C(52)-C(51)-H(51)	117.7(9)		
C(53)-C(52)-C(51)	120.03(11)		
C(53)-C(52)-H(52)	120.2(9)		
C(51)-C(52)-H(52)	119.7(9)		
C(54)-C(53)-C(52)	119.94(10)		
C(54)-C(53)-H(53)	121.8(9)		
C(52)-C(53)-H(53)	118.2(9)		
C(53)-C(54)-C(55)	120.04(10)		
C(53)-C(54)-H(54)	121.3(9)		
C(55)-C(54)-H(54)	118.7(9)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1

Table S18. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	60(1)	81(1)	69(1)	3(1)	-12(1)	-6(1)
S(1)	86(1)	122(1)	100(1)	-13(1)	-25(1)	-13(1)
F(1)	416(4)	293(4)	753(6)	266(4)	-402(4)	-110(3)
F(2)	314(4)	456(4)	658(6)	-377(4)	-247(4)	228(3)
F(3)	186(3)	310(3)	457(4)	-34(3)	-215(3)	-17(2)
O(1)	88(2)	94(2)	123(3)	-14(2)	-28(2)	-2(2)
O(2)	116(2)	93(2)	90(2)	-5(2)	-23(2)	15(2)
O(3)	112(2)	124(2)	128(3)	15(2)	-61(2)	-26(2)
O(4)	161(3)	246(3)	163(3)	61(3)	-50(2)	-94(2)
O(5)	178(3)	302(4)	158(3)	-112(3)	-19(2)	-43(3)
N(1)	73(2)	81(2)	89(3)	0(2)	-18(2)	-1(2)
C(1)	96(3)	90(3)	98(3)	5(2)	-26(2)	0(2)
C(2)	128(3)	90(3)	127(3)	4(3)	-39(3)	-9(2)
C(3)	150(3)	88(3)	156(4)	0(3)	-44(3)	8(2)
C(4)	113(3)	105(3)	130(3)	2(3)	-26(3)	20(2)
C(5)	93(3)	101(3)	129(3)	7(3)	-17(3)	2(2)
C(6)	99(3)	81(3)	103(3)	5(2)	-19(2)	1(2)
C(7)	80(3)	86(3)	100(3)	-2(2)	-21(2)	1(2)
C(8)	84(3)	99(3)	113(3)	5(2)	-11(2)	7(2)
C(9)	85(3)	107(3)	92(3)	1(2)	-16(2)	-6(2)
C(10)	94(3)	92(3)	111(3)	13(2)	-17(2)	-1(2)

C(11)	91(3)	84(3)	88(3)	0(2)	-21(2)	4(2)
C(12)	80(3)	88(3)	106(3)	2(2)	-22(2)	3(2)
C(13)	104(3)	109(3)	111(3)	6(3)	-22(3)	4(2)
C(14)	114(3)	106(3)	133(3)	13(3)	-41(3)	6(2)
C(15)	103(3)	105(3)	148(4)	-3(3)	-37(3)	17(2)
C(16)	80(3)	95(3)	123(3)	-18(2)	-23(2)	4(2)
C(17)	82(3)	89(3)	105(3)	-3(2)	-27(2)	-8(2)
C(18)	154(3)	98(3)	165(4)	6(3)	-58(3)	-29(3)
C(19)	271(5)	162(4)	232(5)	2(3)	-153(4)	-45(3)
C(20)	187(4)	184(4)	205(5)	10(3)	-35(3)	-81(3)
C(21)	228(4)	100(3)	344(6)	-14(4)	-98(4)	-30(3)
C(22)	125(3)	132(3)	149(4)	-2(3)	-27(3)	42(3)
C(23)	252(5)	436(7)	206(5)	-66(5)	-106(4)	141(5)
C(24)	134(4)	189(4)	270(5)	18(4)	-7(3)	21(3)
C(25)	187(4)	134(4)	391(7)	11(4)	-57(4)	53(3)
C(26)	88(3)	121(3)	113(3)	18(3)	-4(2)	-9(2)
C(27)	124(3)	186(4)	170(4)	37(3)	36(3)	27(3)
C(28)	139(4)	211(4)	199(4)	-5(3)	-41(3)	-61(3)
C(29)	149(4)	181(4)	120(4)	39(3)	-19(3)	-8(3)
C(30)	157(4)	161(4)	145(4)	23(3)	-49(3)	42(3)
C(31)	258(5)	273(5)	219(5)	39(4)	-75(4)	133(4)
C(32)	245(5)	266(5)	250(5)	135(4)	-42(4)	-5(4)
C(33)	357(6)	277(5)	217(5)	-31(4)	-175(5)	66(4)
C(34)	94(3)	119(3)	131(3)	-30(3)	-18(3)	13(2)
C(35)	138(3)	166(4)	162(4)	-60(3)	-49(3)	13(3)
C(36)	131(3)	133(3)	207(4)	-49(3)	-32(3)	39(3)
C(37)	107(3)	163(4)	160(4)	-14(3)	-13(3)	-8(3)
C(38)	181(4)	193(4)	354(6)	-34(4)	-171(4)	12(3)
C(39)	105(3)	134(3)	107(3)	-13(3)	-44(3)	-11(2)

C(40)	102(3)	136(3)	97(3)	2(3)	-41(3)	-9(2)
C(41)	130(3)	136(3)	120(3)	24(3)	-48(3)	-6(3)
C(42)	137(3)	163(4)	119(4)	45(3)	-34(3)	-23(3)
C(43)	92(3)	144(3)	106(3)	25(3)	-11(3)	-30(2)
C(44)	81(3)	159(3)	94(3)	6(3)	-1(2)	-10(2)
C(45)	115(3)	175(4)	103(3)	-17(3)	-4(3)	7(3)
C(46)	142(3)	196(4)	114(3)	-42(3)	-37(3)	-3(3)
C(51)	192(4)	306(5)	239(5)	41(4)	-66(4)	-36(4)
C(52)	279(5)	295(5)	207(5)	-11(4)	-100(4)	-35(4)
C(53)	223(4)	179(4)	307(6)	10(4)	-144(4)	-40(3)
C(54)	180(4)	216(4)	307(6)	-22(4)	-98(4)	17(3)
C(55)	239(4)	202(4)	259(5)	-49(4)	-125(4)	44(3)
C(56)	200(4)	199(4)	292(5)	31(4)	-137(4)	-24(3)
C(61)	199(4)	205(4)	166(4)	-16(3)	-40(3)	-19(3)
C(62)	184(4)	227(4)	123(4)	-23(3)	-10(3)	-62(3)
C(63)	159(4)	226(4)	166(4)	-54(3)	-12(3)	-23(3)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **7**.

	x	y	z	U_{iso}
H(3)	11025(10)	1189(9)	7559(8)	12(3)
H(5)	12471(9)	3933(8)	7258(7)	6(2)
H(8)	12291(9)	4973(8)	6328(7)	9(3)
H(10)	10528(10)	7680(9)	6236(8)	13(3)
H(13)	8864(9)	7646(8)	5899(8)	10(3)
H(15)	6038(10)	9218(9)	7323(8)	16(3)
H(19A)	7508(12)	1564(11)	7034(9)	32(4)
H(19B)	8728(12)	1938(11)	6495(10)	29(4)
H(19C)	7855(11)	2654(11)	7068(9)	24(3)
H(20A)	7116(12)	1234(11)	8563(9)	29(4)
H(20B)	7420(11)	2366(10)	8598(9)	25(3)
H(20C)	8088(12)	1513(11)	8967(9)	30(4)
H(21A)	9424(11)	229(10)	8026(9)	25(3)
H(21B)	9720(12)	452(10)	7055(9)	28(3)
H(21C)	8433(12)	110(10)	7597(9)	27(3)
H(23A)	12748(12)	1822(11)	8685(9)	27(3)
H(23B)	13353(12)	2940(12)	8349(10)	35(4)
H(23C)	14123(13)	1853(12)	8317(10)	39(4)
H(24A)	14915(12)	2113(11)	6800(9)	30(4)
H(24B)	14246(11)	3151(11)	6831(9)	25(3)
H(24C)	14078(13)	2332(12)	6221(10)	38(4)
H(25A)	14007(12)	538(11)	7357(9)	30(4)
H(25B)	13047(12)	671(11)	6884(10)	30(4)
H(25C)	12618(12)	473(11)	7814(10)	32(4)
H(27A)	14052(10)	5738(9)	5721(8)	16(3)

H(27B)	14464(11)	6365(9)	4854(8)	19(3)
H(27C)	13545(11)	5533(10)	4998(9)	23(3)
H(28A)	12643(11)	8211(10)	6166(8)	21(3)
H(28B)	13958(11)	7996(10)	5576(9)	26(3)
H(28C)	13469(11)	7396(10)	6441(9)	24(3)
H(29A)	12152(11)	6864(10)	4580(9)	26(3)
H(29B)	13169(11)	7612(9)	4429(8)	20(3)
H(29C)	11852(11)	7923(10)	5009(9)	24(3)
H(31A)	5439(12)	9473(11)	6160(9)	28(3)
H(31B)	6088(13)	10126(12)	5373(10)	40(4)
H(31C)	6251(11)	10326(11)	6228(9)	28(4)
H(32A)	8475(13)	10141(12)	5592(11)	42(4)
H(32B)	8298(13)	9942(12)	4753(11)	41(4)
H(32C)	9085(13)	9168(11)	5087(10)	34(4)
H(33A)	7671(13)	7757(12)	4997(10)	35(4)
H(33B)	6891(13)	8558(12)	4666(11)	41(4)
H(33C)	6310(13)	7861(11)	5433(10)	35(4)
H(35A)	7231(10)	8054(9)	9433(8)	16(3)
H(35B)	6243(11)	8841(10)	9900(9)	25(3)
H(35C)	7272(11)	9222(10)	9123(9)	23(3)
H(36A)	5773(11)	10058(10)	8498(9)	23(3)
H(36B)	4794(11)	9674(10)	9316(9)	26(3)
H(36C)	4670(10)	9425(9)	8459(8)	18(3)
H(37A)	4434(11)	7688(9)	8926(8)	19(3)
H(37B)	4588(11)	7851(10)	9799(9)	22(3)
H(37C)	5379(10)	7028(9)	9228(8)	14(3)
H(39)	9428(9)	6245(8)	9029(7)	7(2)
H(40)	10209(9)	4701(8)	8670(7)	5(2)
H(41A)	9373(9)	3667(8)	9987(7)	11(3)

H(41B)	9320(10)	3191(9)	9210(8)	11(3)
H(42A)	7415(10)	2971(9)	10009(8)	13(3)
H(42B)	7375(10)	3955(9)	10457(8)	14(3)
H(43)	6655(9)	3822(9)	9078(7)	10(3)
H(44)	5902(10)	5417(9)	9251(8)	14(3)
H(45A)	6219(11)	5607(10)	10648(9)	21(3)
H(45B)	6423(10)	6502(9)	10064(7)	11(3)
H(46A)	8157(10)	6566(10)	10237(8)	18(3)
H(46B)	8212(10)	5439(9)	10523(8)	16(3)
H(51)	2985(13)	8261(11)	8103(10)	32(4)
H(52)	1405(13)	7789(12)	7681(10)	37(4)
H(53)	-554(12)	8013(11)	8479(9)	30(4)
H(54)	-1000(12)	8687(11)	9783(9)	31(4)
H(55)	592(12)	9151(11)	10214(10)	31(4)
H(56)	2542(12)	8969(10)	9406(9)	28(3)
H(61)	10729(11)	3554(10)	5596(9)	24(3)
H(62)	8876(11)	4301(10)	6253(9)	21(3)
H(63)	8120(11)	5741(10)	5681(8)	21(3)

(ONO^{tBu})Ir(PPh_3)$_2$OTf, 8

Crystals were mounted on a glass fiber using Paratone oil, then placed on the diffractometer under a nitrogen stream at 100K.

The asymmetric contains two distinct sites containing solvent. One site is wholly occupied by benzene with ideal hexagonal geometry imposed during least-squares. The other site contains a mixture of pentane and benzene and was refined without restraints.

One tertiary butyl group, on the pyridine, is disordered and was refined with the limit on total occupancy set to unity.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **8**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ir(1)	7371(1)	7533(1)	9138(1)	12(1)	1
S(1)	4776(1)	7749(1)	8428(1)	40(1)	1
P(1)	8089(1)	7426(1)	8364(1)	16(1)	1
P(2)	6683(1)	7603(1)	9926(1)	14(1)	1
F(1)	3062(2)	7374(1)	7817(1)	59(1)	1
F(2)	3864(2)	6729(1)	8367(1)	55(1)	1
F(3)	4471(2)	6944(1)	7696(1)	70(1)	1
O(1)	7222(2)	6663(1)	9276(1)	16(1)	1
O(2)	7468(2)	8402(1)	8974(1)	16(1)	1
O(3)	5828(2)	7486(1)	8595(1)	21(1)	1
O(4)	4272(2)	7867(1)	8859(1)	60(1)	1
O(5)	4674(3)	8208(2)	8034(2)	69(1)	1
N(1)	8828(2)	7537(1)	9612(1)	13(1)	1
C(1)	8015(3)	6303(1)	9273(1)	15(1)	1
C(2)	7800(3)	5703(1)	9143(1)	17(1)	1
C(3)	8634(3)	5355(1)	9089(1)	18(1)	1
C(4)	9673(3)	5548(1)	9150(1)	17(1)	1
C(5)	9876(3)	6113(1)	9313(1)	17(1)	1

C(6)	9076(2)	6492(1)	9399(1)	14(1)	1
C(7)	9442(3)	7047(1)	9676(1)	16(1)	1
C(8)	10425(3)	7054(1)	10027(1)	19(1)	1
C(9)	10870(2)	7552(1)	10282(1)	20(1)	1
C(10)	10240(3)	8043(1)	10189(1)	19(1)	1
C(11)	9219(2)	8036(1)	9882(1)	15(1)	1
C(12)	8591(2)	8579(1)	9837(1)	15(1)	1
C(13)	8831(2)	8961(1)	10276(1)	16(1)	1
C(14)	8472(3)	9520(1)	10254(1)	17(1)	1
C(15)	7934(3)	9724(1)	9752(1)	18(1)	1
C(16)	7671(3)	9377(1)	9305(1)	17(1)	1
C(17)	7900(2)	8768(1)	9362(1)	15(1)	1
C(18)	6681(3)	5452(1)	9080(1)	20(1)	1
C(19)	6415(3)	5476(1)	9629(1)	24(1)	1
C(20)	5840(3)	5787(1)	8667(1)	24(1)	1
C(21)	6616(3)	4814(1)	8904(2)	28(1)	1
C(22)	10530(3)	5136(1)	9039(1)	21(1)	1
C(23)	10234(3)	4942(2)	8458(1)	32(1)	1
C(24)	10630(3)	4598(2)	9402(2)	31(1)	1
C(25)	11620(3)	5429(2)	9143(2)	32(1)	1
C(26)	11970(3)	7566(2)	10640(2)	29(1)	1
C(27)	12468(6)	6940(3)	10743(3)	44(2)	0.691(7)
C(28)	11881(5)	7783(3)	11213(2)	39(2)	0.691(7)
C(29)	12646(5)	7949(4)	10425(3)	54(2)	0.691(7)
C(27B)	12772(10)	7512(7)	10191(6)	47(4)	0.309(7)
C(28B)	12177(15)	7122(8)	10964(9)	62(6)	0.309(7)
C(29B)	12311(10)	8197(6)	10836(6)	48(5)	0.309(7)
C(30)	8670(3)	9930(1)	10736(1)	22(1)	1
C(31)	9301(3)	10462(1)	10621(2)	31(1)	1

C(32)	7598(3)	10129(2)	10833(2)	41(1)	1
C(33)	9295(3)	9628(1)	11237(1)	28(1)	1
C(34)	7200(3)	9648(1)	8751(1)	21(1)	1
C(35)	7168(3)	10317(1)	8776(1)	27(1)	1
C(36)	7939(3)	9484(1)	8389(1)	22(1)	1
C(37)	6067(3)	9440(2)	8509(1)	26(1)	1
C(38)	7610(3)	6786(1)	7955(1)	19(1)	1
C(39)	6715(3)	6849(2)	7536(2)	27(1)	1
C(40)	6299(3)	6371(2)	7235(2)	33(1)	1
C(41)	6745(3)	5828(2)	7332(1)	28(1)	1
C(42)	7630(3)	5763(1)	7740(1)	23(1)	1
C(43)	8050(3)	6236(1)	8054(1)	20(1)	1
C(44)	7787(3)	8005(1)	7866(1)	22(1)	1
C(45)	8521(3)	8170(2)	7577(2)	32(1)	1
C(46)	8251(4)	8576(2)	7165(2)	39(1)	1
C(47)	7262(3)	8809(2)	7041(2)	36(1)	1
C(48)	6516(3)	8651(2)	7322(2)	32(1)	1
C(49)	6793(3)	8252(1)	7741(1)	26(1)	1
C(50)	9537(3)	7441(1)	8515(1)	18(1)	1
C(51)	10184(3)	7021(2)	8359(1)	24(1)	1
C(52)	11264(3)	7089(2)	8491(2)	31(1)	1
C(53)	11730(3)	7561(2)	8781(2)	31(1)	1
C(54)	11094(3)	7984(2)	8925(1)	27(1)	1
C(55)	10016(3)	7927(1)	8794(1)	23(1)	1
C(56)	5781(3)	7017(1)	10012(1)	18(1)	1
C(57)	5029(3)	6821(2)	9583(2)	30(1)	1
C(58)	4283(3)	6410(2)	9645(2)	34(1)	1
C(59)	4290(3)	6184(2)	10132(2)	31(1)	1
C(60)	5039(3)	6369(2)	10565(2)	36(1)	1

C(61)	5792(3)	6785(2)	10514(2)	28(1)	1
C(62)	5926(2)	8240(1)	10034(1)	17(1)	1
C(63)	5653(3)	8670(1)	9648(1)	21(1)	1
C(64)	5052(3)	9147(1)	9728(1)	26(1)	1
C(65)	4738(3)	9207(2)	10196(2)	28(1)	1
C(66)	5007(3)	8782(2)	10586(1)	25(1)	1
C(67)	5584(3)	8300(2)	10504(1)	23(1)	1
C(68)	7711(2)	7529(1)	10540(1)	16(1)	1
C(69)	8270(3)	7004(1)	10632(1)	22(1)	1
C(70)	9028(3)	6911(2)	11102(1)	27(1)	1
C(71)	9230(3)	7343(2)	11489(2)	30(1)	1
C(72)	8696(3)	7867(2)	11396(1)	28(1)	1
C(73)	7951(3)	7964(1)	10930(1)	20(1)	1
C(74)	4047(4)	7167(2)	8071(2)	46(1)	1
C(81)	6954(6)	6302(3)	2632(2)	298(10)	1
C(82)	7439(5)	6304(3)	2207(3)	188(5)	1
C(83)	7157(5)	5891(3)	1806(2)	123(3)	1
C(84)	6389(5)	5478(3)	1830(2)	174(5)	1
C(85)	5904(4)	5476(3)	2255(3)	163(4)	1
C(86)	6186(5)	5888(3)	2656(2)	138(3)	1
C(91)	6761(13)	8607(13)	2064(7)	105(9)	0.471(10)
C(92)	6218(12)	8052(8)	1936(5)	60(4)	0.471(10)
C(93)	5133(10)	8027(6)	1901(5)	26(3)	0.471(10)
C(94)	4578(9)	8501(6)	2031(4)	46(3)	0.471(10)
C(95)	5059(13)	9001(8)	2159(5)	56(4)	0.471(10)
C(96)	6170(14)	9073(15)	2182(10)	74(7)	0.471(10)

C(91B)	6627(14)	9531(7)	2263(6)	139(7)	0.529(10)
C(92B)	5658(14)	9098(9)	2132(7)	65(5)	0.529(10)
C(93B)	6099(14)	8517(7)	2077(5)	80(5)	0.529(10)
C(94B)	5180(30)	8048(17)	1936(11)	175(14)	0.529(10)
C(95B)	5547(11)	7439(7)	1889(5)	84(5)	0.529(10)

Table S21. Selected bond lengths [Å] and angles [°] for **8**.

Ir(1)-N(1)	2.001(3)	N(1)-Ir(1)-O(1)	90.68(9)
Ir(1)-O(1)	2.049(2)	N(1)-Ir(1)-O(2)	91.55(9)
Ir(1)-O(2)	2.051(2)	O(1)-Ir(1)-O(2)	177.70(8)
Ir(1)-O(3)	2.166(2)	N(1)-Ir(1)-O(3)	176.28(9)
Ir(1)-P(1)	2.4142(8)	O(1)-Ir(1)-O(3)	87.33(8)
Ir(1)-P(2)	2.4165(8)	O(2)-Ir(1)-O(3)	90.41(8)
		N(1)-Ir(1)-P(1)	90.90(7)
		O(1)-Ir(1)-P(1)	96.69(6)
		O(2)-Ir(1)-P(1)	82.71(6)
		O(3)-Ir(1)-P(1)	86.22(6)
		N(1)-Ir(1)-P(2)	88.06(7)
		O(1)-Ir(1)-P(2)	81.27(6)
		O(2)-Ir(1)-P(2)	99.37(6)
		O(3)-Ir(1)-P(2)	94.74(6)
		P(1)-Ir(1)-P(2)	177.70(3)

Table S22. Bond lengths [Å] and angles [°] for **8.**

Ir(1)-N(1)	2.001(3)	C(3)-C(4)	1.395(4)
Ir(1)-O(1)	2.049(2)	C(4)-C(5)	1.374(4)
Ir(1)-O(2)	2.051(2)	C(4)-C(22)	1.538(4)
Ir(1)-O(3)	2.166(2)	C(5)-C(6)	1.413(4)
Ir(1)-P(1)	2.4142(8)	C(6)-C(7)	1.486(4)
Ir(1)-P(2)	2.4165(8)	C(7)-C(8)	1.384(4)
S(1)-O(4)	1.446(3)	C(8)-C(9)	1.378(4)
S(1)-O(5)	1.453(3)	C(9)-C(10)	1.382(4)
S(1)-O(3)	1.464(2)	C(9)-C(26)	1.511(5)
S(1)-C(74)	1.769(5)	C(10)-C(11)	1.378(4)
P(1)-C(50)	1.831(3)	C(11)-C(12)	1.482(4)
P(1)-C(44)	1.831(3)	C(12)-C(17)	1.411(4)
P(1)-C(38)	1.833(3)	C(12)-C(13)	1.412(4)
P(2)-C(62)	1.822(3)	C(13)-C(14)	1.364(4)
P(2)-C(68)	1.830(3)	C(14)-C(15)	1.404(4)
P(2)-C(56)	1.833(3)	C(14)-C(30)	1.538(4)
F(1)-C(74)	1.380(5)	C(15)-C(16)	1.382(4)
F(2)-C(74)	1.320(5)	C(16)-C(17)	1.430(4)
F(3)-C(74)	1.326(5)	C(16)-C(34)	1.553(4)
O(1)-C(1)	1.323(3)	C(18)-C(21)	1.533(4)
O(2)-C(17)	1.331(4)	C(18)-C(19)	1.540(5)
N(1)-C(7)	1.367(4)	C(18)-C(20)	1.545(5)
N(1)-C(11)	1.376(4)	C(22)-C(23)	1.530(5)
C(1)-C(6)	1.410(4)	C(22)-C(25)	1.533(5)
C(1)-C(2)	1.432(4)	C(22)-C(24)	1.542(5)
C(2)-C(3)	1.381(4)	C(26)-C(28B)	1.309(18)
C(2)-C(18)	1.537(5)	C(26)-C(29)	1.442(7)

C(26)-C(29B)	1.566(14)	C(56)-C(61)	1.401(5)
C(26)-C(27)	1.576(8)	C(57)-C(58)	1.389(5)
C(26)-C(28)	1.595(7)	C(58)-C(59)	1.362(5)
C(26)-C(27B)	1.736(15)	C(59)-C(60)	1.369(5)
C(30)-C(33)	1.526(5)	C(60)-C(61)	1.396(5)
C(30)-C(31)	1.539(5)	C(62)-C(63)	1.391(4)
C(30)-C(32)	1.542(5)	C(62)-C(67)	1.396(4)
C(34)-C(37)	1.535(5)	C(63)-C(64)	1.389(4)
C(34)-C(35)	1.539(4)	C(64)-C(65)	1.371(5)
C(34)-C(36)	1.537(4)	C(65)-C(66)	1.390(5)
C(38)-C(43)	1.387(4)	C(66)-C(67)	1.382(4)
C(38)-C(39)	1.401(5)	C(68)-C(69)	1.400(4)
C(39)-C(40)	1.383(5)	C(68)-C(73)	1.404(4)
C(40)-C(41)	1.374(5)	C(69)-C(70)	1.391(5)
C(41)-C(42)	1.376(5)	C(70)-C(71)	1.392(5)
C(42)-C(43)	1.390(4)	C(71)-C(72)	1.383(5)
C(44)-C(49)	1.378(5)	C(72)-C(73)	1.379(5)
C(44)-C(45)	1.395(5)	C(81)-C(82)	1.3900
C(45)-C(46)	1.400(5)	C(81)-C(86)	1.3900
C(46)-C(47)	1.359(6)	C(82)-C(83)	1.3900
C(47)-C(48)	1.388(5)	C(83)-C(84)	1.3900
C(48)-C(49)	1.403(5)	C(84)-C(85)	1.3900
C(50)-C(55)	1.395(4)	C(85)-C(86)	1.3900
C(50)-C(51)	1.400(4)	C(91)-C(96)	1.39(4)
C(51)-C(52)	1.374(5)	C(91)-C(92)	1.46(3)
C(52)-C(53)	1.377(5)	C(92)-C(93)	1.39(2)
C(53)-C(54)	1.382(5)	C(93)-C(94)	1.390(18)
C(54)-C(55)	1.368(5)	C(94)-C(95)	1.31(2)
C(56)-C(57)	1.373(5)	C(95)-C(96)	1.44(2)

C(91B)-C(92B)	1.58(2)	C(50)-P(1)-Ir(1)	113.41(11)
C(92B)-C(93B)	1.47(3)	C(44)-P(1)-Ir(1)	116.77(11)
C(93B)-C(94B)	1.58(3)	C(38)-P(1)-Ir(1)	114.65(11)
C(94B)-C(95B)	1.49(3)	C(62)-P(2)-C(68)	104.65(15)
		C(62)-P(2)-C(56)	100.85(15)
N(1)-Ir(1)-O(1)	90.68(9)	C(68)-P(2)-C(56)	100.53(15)
N(1)-Ir(1)-O(2)	91.55(9)	C(62)-P(2)-Ir(1)	120.19(11)
O(1)-Ir(1)-O(2)	177.70(8)	C(68)-P(2)-Ir(1)	112.82(10)
N(1)-Ir(1)-O(3)	176.28(9)	C(56)-P(2)-Ir(1)	115.31(11)
O(1)-Ir(1)-O(3)	87.33(8)	C(1)-O(1)-Ir(1)	120.21(19)
O(2)-Ir(1)-O(3)	90.41(8)	C(17)-O(2)-Ir(1)	119.70(19)
N(1)-Ir(1)-P(1)	90.90(7)	S(1)-O(3)-Ir(1)	146.06(15)
O(1)-Ir(1)-P(1)	96.69(6)	C(7)-N(1)-C(11)	119.2(3)
O(2)-Ir(1)-P(1)	82.71(6)	C(7)-N(1)-Ir(1)	120.8(2)
O(3)-Ir(1)-P(1)	86.22(6)	C(11)-N(1)-Ir(1)	120.0(2)
N(1)-Ir(1)-P(2)	88.06(7)	O(1)-C(1)-C(6)	121.9(3)
O(1)-Ir(1)-P(2)	81.27(6)	O(1)-C(1)-C(2)	119.6(3)
O(2)-Ir(1)-P(2)	99.37(6)	C(6)-C(1)-C(2)	118.5(3)
O(3)-Ir(1)-P(2)	94.74(6)	C(3)-C(2)-C(1)	117.9(3)
P(1)-Ir(1)-P(2)	177.70(3)	C(3)-C(2)-C(18)	121.1(3)
O(4)-S(1)-O(5)	115.0(2)	C(1)-C(2)-C(18)	121.0(3)
O(4)-S(1)-O(3)	114.16(18)	C(2)-C(3)-C(4)	124.5(3)
O(5)-S(1)-O(3)	115.68(18)	C(5)-C(4)-C(3)	116.5(3)
O(4)-S(1)-C(74)	105.1(2)	C(5)-C(4)-C(22)	122.9(3)
O(5)-S(1)-C(74)	103.4(2)	C(3)-C(4)-C(22)	120.5(3)
O(3)-S(1)-C(74)	101.06(19)	C(4)-C(5)-C(6)	122.4(3)
C(50)-P(1)-C(44)	100.19(15)	C(1)-C(6)-C(5)	119.4(3)
C(50)-P(1)-C(38)	109.41(15)	C(1)-C(6)-C(7)	124.1(3)
C(44)-P(1)-C(38)	100.84(16)	C(5)-C(6)-C(7)	116.2(3)

N(1)-C(7)-C(8)	119.6(3)	C(2)-C(18)-C(20)	112.7(3)
N(1)-C(7)-C(6)	122.4(3)	C(19)-C(18)-C(20)	110.3(3)
C(8)-C(7)-C(6)	118.0(3)	C(23)-C(22)-C(25)	108.2(3)
C(9)-C(8)-C(7)	122.9(3)	C(23)-C(22)-C(4)	109.6(3)
C(8)-C(9)-C(10)	115.4(3)	C(25)-C(22)-C(4)	112.2(3)
C(8)-C(9)-C(26)	122.9(3)	C(23)-C(22)-C(24)	109.4(3)
C(10)-C(9)-C(26)	121.8(3)	C(25)-C(22)-C(24)	107.5(3)
C(11)-C(10)-C(9)	122.8(3)	C(4)-C(22)-C(24)	109.9(3)
N(1)-C(11)-C(10)	119.6(3)	C(28B)-C(26)-C(29)	132.0(10)
N(1)-C(11)-C(12)	122.1(3)	C(28B)-C(26)-C(9)	113.5(8)
C(10)-C(11)-C(12)	118.3(3)	C(29)-C(26)-C(9)	110.6(4)
C(17)-C(12)-C(13)	119.1(3)	C(28B)-C(26)-C(29B)	120.9(11)
C(17)-C(12)-C(11)	123.7(3)	C(29)-C(26)-C(29B)	53.8(7)
C(13)-C(12)-C(11)	116.5(3)	C(9)-C(26)-C(29B)	112.0(5)
C(14)-C(13)-C(12)	122.8(3)	C(28B)-C(26)-C(27)	33.3(12)
C(13)-C(14)-C(15)	116.4(3)	C(29)-C(26)-C(27)	111.0(5)
C(13)-C(14)-C(30)	123.5(3)	C(9)-C(26)-C(27)	112.1(4)
C(15)-C(14)-C(30)	120.0(3)	C(29B)-C(26)-C(27)	135.8(6)
C(16)-C(15)-C(14)	123.8(3)	C(28B)-C(26)-C(28)	72.3(11)
C(15)-C(16)-C(17)	118.2(3)	C(29)-C(26)-C(28)	110.5(5)
C(15)-C(16)-C(34)	120.7(3)	C(9)-C(26)-C(28)	108.2(3)
C(17)-C(16)-C(34)	121.1(3)	C(29B)-C(26)-C(28)	59.0(7)
O(2)-C(17)-C(12)	122.2(3)	C(27)-C(26)-C(28)	104.2(4)
O(2)-C(17)-C(16)	120.0(3)	C(28B)-C(26)-C(27B)	107.9(12)
C(12)-C(17)-C(16)	117.8(3)	C(29)-C(26)-C(27B)	43.3(5)
C(21)-C(18)-C(2)	112.1(3)	C(9)-C(26)-C(27B)	102.6(5)
C(21)-C(18)-C(19)	107.4(3)	C(29B)-C(26)-C(27B)	96.6(8)
C(2)-C(18)-C(19)	107.4(3)	C(27)-C(26)-C(27B)	76.2(6)
C(21)-C(18)-C(20)	106.9(3)	C(28)-C(26)-C(27B)	146.1(6)

C(33)-C(30)-C(14)	111.5(3)	C(55)-C(50)-P(1)	116.0(2)
C(33)-C(30)-C(31)	108.9(3)	C(51)-C(50)-P(1)	125.5(3)
C(14)-C(30)-C(31)	109.0(3)	C(52)-C(51)-C(50)	119.8(3)
C(33)-C(30)-C(32)	108.6(3)	C(51)-C(52)-C(53)	121.2(3)
C(14)-C(30)-C(32)	109.1(3)	C(52)-C(53)-C(54)	119.1(3)
C(31)-C(30)-C(32)	109.7(3)	C(55)-C(54)-C(53)	120.6(3)
C(37)-C(34)-C(35)	107.1(3)	C(54)-C(55)-C(50)	120.8(3)
C(37)-C(34)-C(36)	110.5(3)	C(57)-C(56)-C(61)	118.4(3)
C(35)-C(34)-C(36)	107.3(3)	C(57)-C(56)-P(2)	119.8(3)
C(37)-C(34)-C(16)	112.7(3)	C(61)-C(56)-P(2)	121.7(3)
C(35)-C(34)-C(16)	111.8(3)	C(56)-C(57)-C(58)	121.0(4)
C(36)-C(34)-C(16)	107.2(3)	C(59)-C(58)-C(57)	120.7(4)
C(43)-C(38)-C(39)	118.0(3)	C(58)-C(59)-C(60)	119.3(4)
C(43)-C(38)-P(1)	123.7(3)	C(59)-C(60)-C(61)	121.0(4)
C(39)-C(38)-P(1)	118.2(2)	C(60)-C(61)-C(56)	119.5(4)
C(40)-C(39)-C(38)	120.0(3)	C(63)-C(62)-C(67)	118.5(3)
C(41)-C(40)-C(39)	121.7(4)	C(63)-C(62)-P(2)	121.1(2)
C(40)-C(41)-C(42)	118.8(3)	C(67)-C(62)-P(2)	120.4(2)
C(41)-C(42)-C(43)	120.5(3)	C(64)-C(63)-C(62)	120.7(3)
C(38)-C(43)-C(42)	121.1(3)	C(65)-C(64)-C(63)	120.3(3)
C(49)-C(44)-C(45)	119.0(3)	C(64)-C(65)-C(66)	119.7(3)
C(49)-C(44)-P(1)	119.9(3)	C(67)-C(66)-C(65)	120.3(3)
C(45)-C(44)-P(1)	120.9(3)	C(66)-C(67)-C(62)	120.5(3)
C(44)-C(45)-C(46)	120.5(4)	C(69)-C(68)-C(73)	118.1(3)
C(47)-C(46)-C(45)	119.9(4)	C(69)-C(68)-P(2)	118.3(2)
C(46)-C(47)-C(48)	120.7(4)	C(73)-C(68)-P(2)	123.5(2)
C(47)-C(48)-C(49)	119.5(4)	C(70)-C(69)-C(68)	121.0(3)
C(44)-C(49)-C(48)	120.4(4)	C(69)-C(70)-C(71)	119.8(3)
C(55)-C(50)-C(51)	118.4(3)	C(72)-C(71)-C(70)	119.6(3)

C(73)-C(72)-C(71)	120.9(3)
C(72)-C(73)-C(68)	120.6(3)
F(2)-C(74)-F(3)	107.0(4)
F(2)-C(74)-F(1)	105.5(4)
F(3)-C(74)-F(1)	106.4(4)
F(2)-C(74)-S(1)	114.8(3)
F(3)-C(74)-S(1)	114.3(3)
F(1)-C(74)-S(1)	108.2(3)
C(82)-C(81)-C(86)	120.0
C(81)-C(82)-C(83)	120.0
C(84)-C(83)-C(82)	120.0
C(85)-C(84)-C(83)	120.0
C(84)-C(85)-C(86)	120.0
C(85)-C(86)-C(81)	120.0
C(96)-C(91)-C(92)	117.4(17)
C(93)-C(92)-C(91)	118.7(15)
C(94)-C(93)-C(92)	121.7(15)
C(95)-C(94)-C(93)	120.3(13)
C(94)-C(95)-C(96)	122(2)
C(91)-C(96)-C(95)	120(3)
C(93B)-C(92B)-C(91B)	106.4(16)
C(92B)-C(93B)-C(94B)	111(2)
C(95B)-C(94B)-C(93B)	115(3)

Table S23. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	121(1)	117(1)	103(1)	-3(1)	4(1)	-4(1)
S(1)	305(6)	466(7)	393(7)	73(5)	21(5)	-17(5)
P(1)	181(4)	172(4)	116(4)	-10(3)	29(3)	-10(3)
P(2)	144(4)	147(4)	119(4)	4(3)	30(3)	9(3)
F(1)	328(14)	900(20)	447(17)	31(14)	-118(12)	33(14)
F(2)	569(18)	580(17)	459(18)	42(13)	50(14)	-68(14)
F(3)	523(18)	1190(30)	390(17)	-299(16)	148(14)	-74(17)
O(1)	178(12)	140(11)	140(12)	9(8)	14(9)	15(9)
O(2)	190(12)	149(11)	107(11)	-21(8)	-23(9)	-19(9)
O(3)	129(10)	278(13)	190(12)	50(10)	-13(9)	30(10)
O(4)	416(19)	770(20)	660(20)	-300(19)	245(18)	-76(17)
O(5)	530(20)	640(20)	840(30)	410(20)	20(20)	-28(18)
N(1)	132(12)	136(13)	126(12)	3(10)	25(9)	5(11)
C(1)	209(17)	148(16)	82(15)	14(11)	33(13)	8(13)
C(2)	232(18)	135(16)	125(16)	8(12)	17(13)	2(13)
C(3)	274(19)	121(16)	143(17)	1(12)	36(14)	-1(13)
C(4)	240(18)	137(16)	136(16)	25(12)	39(14)	48(13)
C(5)	190(17)	182(17)	125(16)	15(12)	7(13)	23(13)
C(6)	190(16)	126(15)	97(15)	8(11)	7(12)	10(12)
C(7)	180(17)	145(16)	132(16)	7(12)	11(13)	1(13)
C(8)	185(17)	193(17)	178(18)	-16(13)	-8(14)	78(14)
C(9)	143(15)	236(18)	189(16)	-72(14)	0(12)	4(14)
C(10)	182(17)	180(17)	168(18)	-54(13)	-21(14)	-39(13)
C(11)	181(16)	134(16)	132(16)	-13(12)	21(13)	-29(12)

C(12)	169(16)	126(15)	149(16)	1(12)	32(13)	-18(12)
C(13)	165(16)	191(17)	110(16)	-7(12)	-11(13)	-19(13)
C(14)	197(17)	157(16)	150(17)	-23(12)	16(13)	-21(13)
C(15)	234(18)	113(16)	204(18)	-4(12)	54(14)	5(13)
C(16)	190(17)	149(16)	166(17)	7(12)	28(13)	-20(13)
C(17)	143(16)	148(16)	158(17)	1(12)	34(13)	-3(12)
C(18)	220(18)	146(16)	225(19)	-31(13)	54(14)	-23(13)
C(19)	261(19)	210(18)	260(20)	14(14)	93(16)	-16(15)
C(20)	233(19)	231(19)	250(20)	-39(14)	19(16)	-49(15)
C(21)	270(20)	178(18)	390(20)	-46(15)	97(18)	-44(15)
C(22)	242(19)	168(17)	199(18)	-27(13)	40(15)	39(14)
C(23)	350(20)	370(20)	250(20)	-72(16)	77(18)	85(17)
C(24)	350(20)	250(20)	310(20)	17(16)	59(18)	89(17)
C(25)	280(20)	260(20)	440(30)	-31(17)	126(19)	73(16)
C(26)	130(16)	320(20)	350(20)	-118(17)	-84(14)	49(16)
C(27)	290(40)	510(50)	400(50)	-230(30)	-160(30)	200(30)
C(28)	260(30)	560(40)	260(30)	-180(30)	-100(20)	130(30)
C(29)	200(30)	930(70)	400(40)	100(40)	-60(30)	-120(40)
C(27B)	160(60)	630(110)	580(100)	-190(80)	-30(60)	50(70)
C(28B)	420(110)	500(130)	670(150)	150(100)	-400(100)	-100(90)
C(29B)	210(70)	450(90)	650(120)	-260(80)	-180(70)	50(60)
C(30)	249(19)	199(18)	191(18)	-60(13)	1(15)	16(14)
C(31)	430(20)	189(19)	260(20)	-44(15)	-54(18)	-34(17)
C(32)	380(20)	560(30)	280(20)	-186(19)	34(19)	130(20)
C(33)	410(20)	212(19)	161(18)	-48(14)	-20(16)	11(16)
C(34)	300(20)	172(17)	138(17)	19(13)	36(14)	20(14)
C(35)	410(20)	204(19)	204(19)	44(14)	63(17)	61(16)
C(36)	300(20)	187(17)	164(18)	22(13)	50(15)	-15(14)
C(37)	270(20)	300(20)	181(19)	64(15)	-7(15)	43(16)

C(38)	250(19)	194(17)	119(16)	-34(12)	26(14)	-12(14)
C(39)	270(20)	240(20)	260(20)	-57(15)	-45(16)	48(16)
C(40)	330(20)	310(20)	280(20)	-100(16)	-73(17)	73(17)
C(41)	320(20)	280(20)	220(20)	-102(15)	13(17)	13(16)
C(42)	280(20)	202(18)	203(19)	-33(14)	42(15)	6(15)
C(43)	249(18)	224(18)	132(17)	-5(13)	30(14)	-25(14)
C(44)	310(20)	185(18)	149(17)	-10(13)	27(15)	-31(15)
C(45)	400(20)	330(20)	230(20)	41(16)	97(18)	3(18)
C(46)	530(30)	410(20)	270(20)	122(18)	160(20)	-10(20)
C(47)	570(30)	300(20)	190(20)	98(16)	33(19)	-10(20)
C(48)	450(30)	230(20)	230(20)	14(15)	-29(18)	26(17)
C(49)	370(20)	204(18)	161(19)	-14(14)	1(16)	-35(16)
C(50)	208(16)	203(17)	154(15)	22(13)	64(12)	-37(14)
C(51)	280(20)	228(19)	240(20)	-8(14)	115(16)	-34(15)
C(52)	260(20)	310(20)	400(20)	5(17)	152(18)	13(16)
C(53)	214(18)	390(20)	350(20)	-10(18)	98(16)	-59(17)
C(54)	250(20)	300(20)	270(20)	-45(15)	59(16)	-81(16)
C(55)	255(19)	239(19)	206(19)	-13(14)	85(15)	-38(15)
C(56)	197(17)	148(16)	220(18)	-1(13)	86(14)	-12(13)
C(57)	330(20)	360(20)	210(20)	-9(16)	68(17)	-127(17)
C(58)	290(20)	400(20)	340(20)	-79(18)	97(18)	-120(18)
C(59)	330(20)	230(20)	420(30)	-32(17)	201(19)	-84(16)
C(60)	400(20)	310(20)	400(30)	90(18)	170(20)	-47(18)
C(61)	340(20)	270(20)	240(20)	42(15)	89(17)	-46(16)
C(62)	158(16)	176(17)	178(17)	-15(13)	23(13)	11(13)
C(63)	229(18)	217(18)	196(18)	-14(13)	58(14)	-14(14)
C(64)	300(20)	210(19)	270(20)	49(14)	90(17)	68(15)
C(65)	300(20)	204(19)	370(20)	-48(15)	118(18)	46(15)
C(66)	280(20)	270(20)	230(20)	-51(15)	106(16)	17(15)

C(67)	270(20)	230(18)	186(18)	13(14)	65(15)	24(15)
C(68)	189(15)	174(16)	119(14)	19(13)	26(11)	-2(13)
C(69)	278(19)	221(18)	163(18)	-3(13)	44(15)	10(15)
C(70)	320(20)	250(20)	210(20)	26(15)	-8(16)	78(16)
C(71)	340(20)	340(20)	172(18)	19(15)	-36(16)	-3(17)
C(72)	370(20)	260(20)	165(19)	-30(14)	-13(16)	-50(17)
C(73)	275(19)	186(17)	138(17)	-8(13)	20(14)	-1(14)
C(74)	510(30)	470(30)	440(30)	60(20)	230(20)	40(20)
C(81)	3900(200)	3430(170)	2360(150)	-1600(130)	2290(150)	-2920(160)
C(82)	2100(110)	2140(110)	1560(100)	-1170(80)	750(90)	-1340(90)
C(83)	920(60)	1600(80)	1130(80)	-230(60)	150(50)	20(60)
C(84)	1460(90)	2180(110)	1660(110)	-770(90)	540(80)	-1050(80)
C(85)	1720(100)	2120(110)	860(70)	-370(70)	-60(70)	-540(80)
C(86)	2110(110)	1380(80)	620(60)	150(50)	230(60)	-20(70)
C(91)	570(100)	2200(300)	470(90)	-40(110)	230(90)	170(140)
C(92)	550(90)	870(110)	360(70)	60(60)	60(60)	50(80)
C(93)	300(60)	360(70)	110(60)	60(50)	10(50)	70(50)
C(94)	530(70)	700(90)	150(50)	60(50)	50(50)	110(60)
C(95)	560(90)	820(110)	240(60)	70(60)	-20(70)	50(90)
C(96)	520(120)	1080(180)	530(110)	-100(90)	-50(110)	-190(150)
C(91B)	1580(170)	1160(140)	1240(150)	-220(100)	-40(120)	-610(120)
C(92B)	660(140)	840(110)	370(80)	-140(60)	-50(120)	-50(150)
C(93B)	1320(160)	640(100)	350(70)	50(60)	20(90)	60(110)
C(94B)	2600(400)	2000(400)	420(150)	-60(170)	-220(190)	-1100(300)
C(95B)	1000(100)	1090(120)	420(70)	40(70)	180(70)	-410(90)

$(ONO^{tBu})Ir(PPh_3)_2OH$, 9

Crystals were mounted on a glass fiber using Paratone oil, then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S24. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **9**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	8700(1)	3369(1)	2749(1)	12(1)
P(1)	7688(1)	4238(1)	2329(1)	14(1)
P(2)	9602(1)	2401(1)	3037(1)	13(1)
O(1)	9683(1)	3362(1)	2124(1)	15(1)
O(2)	7704(1)	3397(1)	3371(1)	13(1)
O(3)	7625(1)	2851(1)	2186(1)	20(1)
N(1)	9778(1)	3874(1)	3310(1)	12(1)
C(1)	10177(1)	3893(1)	2022(1)	15(1)
C(2)	10537(1)	3978(1)	1464(1)	16(1)
C(3)	10915(1)	4569(1)	1343(1)	18(1)
C(4)	10963(1)	5096(1)	1724(1)	18(1)
C(5)	10726(1)	4979(1)	2281(1)	16(1)
C(6)	10396(1)	4382(1)	2450(1)	14(1)
C(7)	10440(1)	4274(1)	3094(1)	13(1)

C(8)	11226(1)	4582(1)	3478(1)	15(1)
C(9)	11321(1)	4524(1)	4090(1)	14(1)
C(10)	10603(1)	4130(1)	4294(1)	14(1)
C(11)	9864(1)	3792(1)	3912(1)	12(1)
C(12)	9146(1)	3380(1)	4176(1)	11(1)
C(13)	9527(1)	3122(1)	4740(1)	13(1)
C(14)	8889(1)	2872(1)	5104(1)	14(1)
C(15)	7817(2)	2942(1)	4909(1)	15(1)
C(16)	7385(1)	3176(1)	4356(1)	14(1)
C(17)	8079(1)	3324(1)	3943(1)	12(1)
C(18)	10543(1)	3419(1)	1028(1)	19(1)
C(19)	9468(2)	3118(1)	844(1)	27(1)
C(20)	11292(2)	2917(1)	1335(1)	27(1)
C(21)	10932(2)	3632(1)	458(1)	26(1)
C(22)	11314(1)	5744(1)	1528(1)	21(1)
C(23)	10657(2)	5934(1)	933(1)	27(1)
C(24)	12459(2)	5710(1)	1453(1)	28(1)
C(25)	11196(2)	6267(1)	1978(1)	27(1)
C(26)	12131(1)	4873(1)	4532(1)	17(1)
C(27)	12856(2)	5275(1)	4222(1)	32(1)
C(28)	11554(2)	5311(1)	4909(1)	26(1)
C(29)	12776(2)	4390(1)	4937(1)	27(1)
C(30)	9303(1)	2559(1)	5701(1)	16(1)
C(31)	8901(2)	1876(1)	5702(1)	22(1)
C(32)	8930(2)	2936(1)	6206(1)	21(1)
C(33)	10488(2)	2537(1)	5814(1)	20(1)
C(34)	6206(1)	3275(1)	4187(1)	16(1)
C(35)	5747(2)	2771(1)	3731(1)	21(1)
C(36)	5660(2)	3227(1)	4735(1)	22(1)

C(37)	5979(2)	3945(1)	3933(1)	20(1)
C(38)	7592(1)	4305(1)	1516(1)	16(1)
C(39)	8348(2)	4616(1)	1260(1)	18(1)
C(40)	8270(2)	4653(1)	643(1)	22(1)
C(41)	7444(2)	4376(1)	279(1)	23(1)
C(42)	6686(2)	4066(1)	529(1)	24(1)
C(43)	6756(2)	4030(1)	1143(1)	20(1)
C(44)	6306(1)	4204(1)	2413(1)	17(1)
C(45)	5769(2)	3629(1)	2375(1)	19(1)
C(46)	4706(2)	3621(1)	2387(1)	24(1)
C(47)	4171(2)	4177(1)	2437(1)	27(1)
C(48)	4706(2)	4748(1)	2486(1)	27(1)
C(49)	5760(2)	4763(1)	2474(1)	23(1)
C(50)	8070(1)	5021(1)	2620(1)	16(1)
C(51)	8040(2)	5567(1)	2271(1)	20(1)
C(52)	8335(2)	6150(1)	2522(1)	23(1)
C(53)	8658(2)	6199(1)	3128(1)	27(1)
C(54)	8663(2)	5668(1)	3485(1)	25(1)
C(55)	8369(2)	5081(1)	3237(1)	19(1)
C(56)	9870(1)	1929(1)	2401(1)	16(1)
C(57)	9019(2)	1727(1)	1996(1)	24(1)
C(58)	9152(2)	1336(1)	1523(1)	30(1)
C(59)	10133(2)	1141(1)	1452(1)	29(1)
C(60)	10979(2)	1331(1)	1853(1)	28(1)
C(61)	10855(2)	1720(1)	2330(1)	21(1)
C(62)	9079(1)	1774(1)	3459(1)	17(1)
C(63)	8197(2)	1862(1)	3716(1)	20(1)
C(64)	7907(2)	1406(1)	4102(1)	28(1)
C(65)	8491(2)	864(1)	4222(1)	31(1)

C(66)	9335(2)	754(1)	3944(1)	30(1)
C(67)	9628(2)	1205(1)	3563(1)	23(1)
C(68)	10891(1)	2529(1)	3475(1)	16(1)
C(69)	11614(2)	2889(1)	3231(1)	20(1)
C(70)	12591(2)	2997(1)	3549(1)	26(1)
C(71)	12861(2)	2749(1)	4116(1)	28(1)
C(72)	12152(2)	2407(1)	4370(1)	24(1)
C(73)	11166(2)	2296(1)	4052(1)	19(1)

Table S25. Selected bond lengths [Å] and angles [°] for **9**.

Ir(1)-N(1)	2.0395(14)	N(1)-Ir(1)-O(3)	179.30(6)
Ir(1)-O(3)	2.0561(13)	N(1)-Ir(1)-O(1)	89.78(5)
Ir(1)-O(1)	2.0624(11)	O(3)-Ir(1)-O(1)	90.03(5)
Ir(1)-O(2)	2.0686(11)	N(1)-Ir(1)-O(2)	89.99(5)
Ir(1)-P(1)	2.3654(5)	O(3)-Ir(1)-O(2)	90.22(5)
Ir(1)-P(2)	2.3920(5)	O(1)-Ir(1)-O(2)	178.69(5)
		N(1)-Ir(1)-P(1)	97.67(4)
		O(3)-Ir(1)-P(1)	83.02(4)
		O(1)-Ir(1)-P(1)	95.33(4)
		O(2)-Ir(1)-P(1)	83.43(4)
		N(1)-Ir(1)-P(2)	90.84(4)
		O(3)-Ir(1)-P(2)	88.46(4)
		O(1)-Ir(1)-P(2)	81.46(4)
		O(2)-Ir(1)-P(2)	99.83(4)
		P(1)-Ir(1)-P(2)	170.911(15)

Table S26. Bond lengths [Å] and angles [°] for **9**.

Ir(1)-N(1)	2.0395(14)	C(6)-C(7)	1.477(2)
Ir(1)-O(3)	2.0561(13)	C(7)-C(8)	1.396(2)
Ir(1)-O(1)	2.0624(11)	C(8)-C(9)	1.383(2)
Ir(1)-O(2)	2.0686(11)	C(8)-H(8)	0.912(17)
Ir(1)-P(1)	2.3654(5)	C(9)-C(10)	1.385(2)
Ir(1)-P(2)	2.3920(5)	C(9)-C(26)	1.526(2)
P(1)-C(50)	1.8189(18)	C(10)-C(11)	1.387(2)
P(1)-C(44)	1.8414(19)	C(10)-H(10)	0.930(17)
P(1)-C(38)	1.8412(17)	C(11)-C(12)	1.472(2)
P(2)-C(62)	1.8282(18)	C(12)-C(13)	1.410(2)
P(2)-C(68)	1.8302(18)	C(12)-C(17)	1.411(2)
P(2)-C(56)	1.8370(18)	C(13)-C(14)	1.370(2)
O(1)-C(1)	1.327(2)	C(13)-H(13)	0.909(17)
O(2)-C(17)	1.3259(18)	C(14)-C(15)	1.404(2)
O(3)-H(1A)	0.79(2)	C(14)-C(30)	1.528(2)
N(1)-C(7)	1.353(2)	C(15)-C(16)	1.387(2)
N(1)-C(11)	1.368(2)	C(15)-H(15)	0.939(17)
C(1)-C(6)	1.416(2)	C(16)-C(17)	1.437(2)
C(1)-C(2)	1.435(2)	C(16)-C(34)	1.536(2)
C(2)-C(3)	1.382(3)	C(18)-C(20)	1.531(3)
C(2)-C(18)	1.540(3)	C(18)-C(19)	1.534(3)
C(3)-C(4)	1.405(3)	C(18)-C(21)	1.535(3)
C(3)-H(3)	0.914(17)	C(19)-H(19A)	0.95(2)
C(4)-C(5)	1.375(2)	C(19)-H(19B)	1.01(2)
C(4)-C(22)	1.530(3)	C(19)-H(19C)	0.96(2)
C(5)-C(6)	1.401(2)	C(20)-H(20A)	1.01(2)
C(5)-H(5)	0.952(18)	C(20)-H(20B)	0.98(2)

C(20)-H(20C)	0.97(2)	C(30)-C(31)	1.533(3)
C(21)-H(21A)	0.97(2)	C(30)-C(32)	1.539(3)
C(21)-H(21B)	0.987(19)	C(31)-H(31A)	0.96(2)
C(21)-H(21C)	0.96(2)	C(31)-H(31B)	0.92(2)
C(22)-C(25)	1.528(3)	C(31)-H(31C)	0.995(19)
C(22)-C(24)	1.529(3)	C(32)-H(32A)	0.96(2)
C(22)-C(23)	1.536(3)	C(32)-H(32B)	0.959(18)
C(23)-H(23A)	0.97(2)	C(32)-H(32C)	0.96(2)
C(23)-H(23B)	0.96(2)	C(33)-H(33A)	0.94(2)
C(23)-H(23C)	0.93(2)	C(33)-H(33B)	0.96(2)
C(24)-H(24A)	0.95(2)	C(33)-H(33C)	0.975(18)
C(24)-H(24B)	1.00(2)	C(34)-C(36)	1.535(3)
C(24)-H(24C)	0.96(2)	C(34)-C(37)	1.535(3)
C(25)-H(25A)	0.95(2)	C(34)-C(35)	1.539(3)
C(25)-H(25B)	0.96(2)	C(35)-H(35A)	0.998(18)
C(25)-H(25C)	0.97(2)	C(35)-H(35B)	0.942(19)
C(26)-C(27)	1.523(3)	C(35)-H(35C)	1.00(2)
C(26)-C(29)	1.532(3)	C(36)-H(36A)	0.99(2)
C(26)-C(28)	1.536(3)	C(36)-H(36B)	0.99(2)
C(27)-H(27A)	1.00(2)	C(36)-H(36C)	0.997(19)
C(27)-H(27B)	0.99(2)	C(37)-H(37A)	0.96(2)
C(27)-H(27C)	0.96(2)	C(37)-H(37B)	0.95(2)
C(28)-H(28A)	0.94(2)	C(37)-H(37C)	0.949(18)
C(28)-H(28B)	0.95(2)	C(38)-C(39)	1.386(3)
C(28)-H(28C)	0.98(2)	C(38)-C(43)	1.396(3)
C(29)-H(29A)	0.96(2)	C(39)-C(40)	1.395(2)
C(29)-H(29B)	0.99(2)	C(39)-H(39)	0.931(18)
C(29)-H(29C)	0.96(2)	C(40)-C(41)	1.379(3)
C(30)-C(33)	1.523(3)	C(40)-H(40)	0.956(18)

C(41)-C(42)	1.381(3)	C(57)-C(58)	1.388(3)
C(41)-H(41)	0.935(19)	C(57)-H(57)	0.921(19)
C(42)-C(43)	1.388(3)	C(58)-C(59)	1.377(3)
C(42)-H(42)	0.91(2)	C(58)-H(58)	0.95(2)
C(43)-H(43)	0.893(17)	C(59)-C(60)	1.374(3)
C(44)-C(49)	1.394(3)	C(59)-H(59)	0.92(2)
C(44)-C(45)	1.395(3)	C(60)-C(61)	1.390(3)
C(45)-C(46)	1.389(3)	C(60)-H(60)	0.92(2)
C(45)-H(45)	0.912(18)	C(61)-H(61)	0.932(19)
C(46)-C(47)	1.378(3)	C(62)-C(63)	1.383(3)
C(46)-H(46)	0.950(18)	C(62)-C(67)	1.395(3)
C(47)-C(48)	1.384(3)	C(63)-C(64)	1.395(3)
C(47)-H(47)	0.883(18)	C(63)-H(63)	0.905(18)
C(48)-C(49)	1.378(3)	C(64)-C(65)	1.375(3)
C(48)-H(48)	0.89(2)	C(64)-H(64)	0.90(2)
C(49)-H(49)	0.941(19)	C(65)-C(66)	1.374(3)
C(50)-C(51)	1.393(3)	C(65)-H(65)	0.95(2)
C(50)-C(55)	1.403(2)	C(66)-C(67)	1.379(3)
C(51)-C(52)	1.383(3)	C(66)-H(66)	0.928(19)
C(51)-H(51)	0.891(19)	C(67)-H(67)	0.885(18)
C(52)-C(53)	1.383(3)	C(68)-C(69)	1.393(3)
C(52)-H(52)	0.94(2)	C(68)-C(73)	1.395(2)
C(53)-C(54)	1.381(3)	C(69)-C(70)	1.378(3)
C(53)-H(53)	0.91(2)	C(69)-H(69)	0.903(19)
C(54)-C(55)	1.387(3)	C(70)-C(71)	1.385(3)
C(54)-H(54)	0.94(2)	C(70)-H(70)	0.92(2)
C(55)-H(55)	0.914(19)	C(71)-C(72)	1.370(3)
C(56)-C(61)	1.388(3)	C(71)-H(71)	0.91(2)
C(56)-C(57)	1.391(3)	C(72)-C(73)	1.388(3)

C(72)-H(72)	0.94(2)	C(56)-P(2)-Ir(1)	113.10(6)
C(73)-H(73)	0.915(17)	C(1)-O(1)-Ir(1)	119.07(11)
		C(17)-O(2)-Ir(1)	119.84(10)
N(1)-Ir(1)-O(3)	179.30(6)	Ir(1)-O(3)-H(1A)	107.9(19)
N(1)-Ir(1)-O(1)	89.78(5)	C(7)-N(1)-C(11)	119.25(14)
O(3)-Ir(1)-O(1)	90.03(5)	C(7)-N(1)-Ir(1)	120.73(11)
N(1)-Ir(1)-O(2)	89.99(5)	C(11)-N(1)-Ir(1)	119.96(11)
O(3)-Ir(1)-O(2)	90.22(5)	O(1)-C(1)-C(6)	122.88(15)
O(1)-Ir(1)-O(2)	178.69(5)	O(1)-C(1)-C(2)	119.72(16)
N(1)-Ir(1)-P(1)	97.67(4)	C(6)-C(1)-C(2)	117.39(17)
O(3)-Ir(1)-P(1)	83.02(4)	C(3)-C(2)-C(1)	117.81(17)
O(1)-Ir(1)-P(1)	95.33(4)	C(3)-C(2)-C(18)	121.41(16)
O(2)-Ir(1)-P(1)	83.43(4)	C(1)-C(2)-C(18)	120.74(16)
N(1)-Ir(1)-P(2)	90.84(4)	C(2)-C(3)-C(4)	124.82(17)
O(3)-Ir(1)-P(2)	88.46(4)	C(2)-C(3)-H(3)	118.8(11)
O(1)-Ir(1)-P(2)	81.46(4)	C(4)-C(3)-H(3)	116.4(11)
O(2)-Ir(1)-P(2)	99.83(4)	C(5)-C(4)-C(3)	115.70(18)
P(1)-Ir(1)-P(2)	170.911(15)	C(5)-C(4)-C(22)	123.44(17)
C(50)-P(1)-C(44)	102.18(8)	C(3)-C(4)-C(22)	120.79(16)
C(50)-P(1)-C(38)	105.52(8)	C(4)-C(5)-C(6)	122.56(18)
C(44)-P(1)-C(38)	101.40(8)	C(4)-C(5)-H(5)	116.9(11)
C(50)-P(1)-Ir(1)	116.86(6)	C(6)-C(5)-H(5)	120.5(11)
C(44)-P(1)-Ir(1)	114.76(6)	C(5)-C(6)-C(1)	120.06(16)
C(38)-P(1)-Ir(1)	114.25(6)	C(5)-C(6)-C(7)	116.52(16)
C(62)-P(2)-C(68)	101.87(8)	C(1)-C(6)-C(7)	122.84(16)
C(62)-P(2)-C(56)	99.05(8)	N(1)-C(7)-C(8)	120.46(15)
C(68)-P(2)-C(56)	103.69(8)	N(1)-C(7)-C(6)	122.13(15)
C(62)-P(2)-Ir(1)	123.55(6)	C(8)-C(7)-C(6)	117.36(16)
C(68)-P(2)-Ir(1)	113.01(6)	C(9)-C(8)-C(7)	121.91(17)

C(9)-C(8)-H(8)	121.4(11)	C(20)-C(18)-C(19)	109.04(19)
C(7)-C(8)-H(8)	116.7(11)	C(20)-C(18)-C(21)	108.38(16)
C(8)-C(9)-C(10)	115.76(16)	C(19)-C(18)-C(21)	107.41(16)
C(8)-C(9)-C(26)	124.26(16)	C(20)-C(18)-C(2)	107.60(15)
C(10)-C(9)-C(26)	119.96(15)	C(19)-C(18)-C(2)	113.25(15)
C(9)-C(10)-C(11)	122.36(16)	C(21)-C(18)-C(2)	111.05(17)
C(9)-C(10)-H(10)	120.3(11)	C(18)-C(19)-H(19A)	109.4(12)
C(11)-C(10)-H(10)	117.3(11)	C(18)-C(19)-H(19B)	111.5(14)
N(1)-C(11)-C(10)	120.05(16)	H(19A)-C(19)-H(19B)	108.8(18)
N(1)-C(11)-C(12)	121.93(15)	C(18)-C(19)-H(19C)	113.0(13)
C(10)-C(11)-C(12)	117.91(15)	H(19A)-C(19)-H(19C)	105.9(18)
C(13)-C(12)-C(17)	119.48(15)	H(19B)-C(19)-H(19C)	108.0(18)
C(13)-C(12)-C(11)	116.48(15)	C(18)-C(20)-H(20A)	111.2(11)
C(17)-C(12)-C(11)	123.15(15)	C(18)-C(20)-H(20B)	109.6(12)
C(14)-C(13)-C(12)	122.76(17)	H(20A)-C(20)-H(20B)	108.0(16)
C(14)-C(13)-H(13)	119.6(11)	C(18)-C(20)-H(20C)	108.7(12)
C(12)-C(13)-H(13)	117.7(11)	H(20A)-C(20)-H(20C)	108.9(16)
C(13)-C(14)-C(15)	115.87(16)	H(20B)-C(20)-H(20C)	110.4(17)
C(13)-C(14)-C(30)	122.83(16)	C(18)-C(21)-H(21A)	112.6(12)
C(15)-C(14)-C(30)	121.25(16)	C(18)-C(21)-H(21B)	110.3(11)
C(16)-C(15)-C(14)	124.28(17)	H(21A)-C(21)-H(21B)	108.9(17)
C(16)-C(15)-H(15)	117.7(10)	C(18)-C(21)-H(21C)	108.6(13)
C(14)-C(15)-H(15)	118.0(10)	H(21A)-C(21)-H(21C)	108.6(17)
C(15)-C(16)-C(17)	117.77(16)	H(21B)-C(21)-H(21C)	107.7(17)
C(15)-C(16)-C(34)	121.22(16)	C(25)-C(22)-C(24)	108.34(18)
C(17)-C(16)-C(34)	121.02(15)	C(25)-C(22)-C(4)	112.41(16)
O(2)-C(17)-C(12)	123.04(14)	C(24)-C(22)-C(4)	109.38(16)
O(2)-C(17)-C(16)	119.78(14)	C(25)-C(22)-C(23)	107.64(18)
C(12)-C(17)-C(16)	117.18(14)	C(24)-C(22)-C(23)	109.18(17)

C(4)-C(22)-C(23)	109.83(16)	H(27A)-C(27)-H(27C)	118.1(17)
C(22)-C(23)-H(23A)	109.5(13)	H(27B)-C(27)-H(27C)	108.3(18)
C(22)-C(23)-H(23B)	111.7(13)	C(26)-C(28)-H(28A)	107.3(14)
H(23A)-C(23)-H(23B)	111.8(18)	C(26)-C(28)-H(28B)	111.3(12)
C(22)-C(23)-H(23C)	109.6(13)	H(28A)-C(28)-H(28B)	109.9(18)
H(23A)-C(23)-H(23C)	107.7(17)	C(26)-C(28)-H(28C)	109.9(12)
H(23B)-C(23)-H(23C)	106.5(18)	H(28A)-C(28)-H(28C)	106.8(19)
C(22)-C(24)-H(24A)	112.6(12)	H(28B)-C(28)-H(28C)	111.5(17)
C(22)-C(24)-H(24B)	111.3(11)	C(26)-C(29)-H(29A)	110.3(13)
H(24A)-C(24)-H(24B)	107.4(16)	C(26)-C(29)-H(29B)	110.8(12)
C(22)-C(24)-H(24C)	109.5(12)	H(29A)-C(29)-H(29B)	109.2(18)
H(24A)-C(24)-H(24C)	105.3(18)	C(26)-C(29)-H(29C)	109.1(13)
H(24B)-C(24)-H(24C)	110.7(16)	H(29A)-C(29)-H(29C)	106.7(17)
C(22)-C(25)-H(25A)	111.2(13)	H(29B)-C(29)-H(29C)	110.7(16)
C(22)-C(25)-H(25B)	109.7(11)	C(33)-C(30)-C(14)	111.60(15)
H(25A)-C(25)-H(25B)	111.2(17)	C(33)-C(30)-C(31)	107.92(16)
C(22)-C(25)-H(25C)	112.3(12)	C(14)-C(30)-C(31)	109.52(15)
H(25A)-C(25)-H(25C)	107.8(17)	C(33)-C(30)-C(32)	108.75(15)
H(25B)-C(25)-H(25C)	104.4(16)	C(14)-C(30)-C(32)	109.48(15)
C(27)-C(26)-C(9)	112.10(15)	C(31)-C(30)-C(32)	109.54(16)
C(27)-C(26)-C(29)	109.11(18)	C(30)-C(31)-H(31A)	111.0(13)
C(9)-C(26)-C(29)	109.41(16)	C(30)-C(31)-H(31B)	110.3(12)
C(27)-C(26)-C(28)	108.63(18)	H(31A)-C(31)-H(31B)	110.1(17)
C(9)-C(26)-C(28)	108.11(15)	C(30)-C(31)-H(31C)	112.2(12)
C(29)-C(26)-C(28)	109.44(17)	H(31A)-C(31)-H(31C)	106.4(17)
C(26)-C(27)-H(27A)	105.7(12)	H(31B)-C(31)-H(31C)	106.8(16)
C(26)-C(27)-H(27B)	109.4(12)	C(30)-C(32)-H(32A)	111.1(12)
H(27A)-C(27)-H(27B)	104.4(16)	C(30)-C(32)-H(32B)	111.7(11)
C(26)-C(27)-H(27C)	110.6(13)	H(32A)-C(32)-H(32B)	106.0(15)

C(30)-C(32)-H(32C)	112.6(11)	H(37A)-C(37)-H(37B)	105.3(16)
H(32A)-C(32)-H(32C)	105.0(16)	C(34)-C(37)-H(37C)	111.8(11)
H(32B)-C(32)-H(32C)	110.1(15)	H(37A)-C(37)-H(37C)	110.3(16)
C(30)-C(33)-H(33A)	111.6(12)	H(37B)-C(37)-H(37C)	111.8(16)
C(30)-C(33)-H(33B)	110.3(12)	C(39)-C(38)-C(43)	118.53(16)
H(33A)-C(33)-H(33B)	106.1(17)	C(39)-C(38)-P(1)	121.36(13)
C(30)-C(33)-H(33C)	111.6(10)	C(43)-C(38)-P(1)	120.10(15)
H(33A)-C(33)-H(33C)	108.5(16)	C(38)-C(39)-C(40)	120.52(18)
H(33B)-C(33)-H(33C)	108.5(16)	C(38)-C(39)-H(39)	120.9(11)
C(16)-C(34)-C(36)	111.31(14)	C(40)-C(39)-H(39)	118.6(11)
C(16)-C(34)-C(37)	110.06(15)	C(41)-C(40)-C(39)	120.46(19)
C(36)-C(34)-C(37)	106.26(16)	C(41)-C(40)-H(40)	120.0(11)
C(16)-C(34)-C(35)	109.87(15)	C(39)-C(40)-H(40)	119.5(11)
C(36)-C(34)-C(35)	108.84(16)	C(40)-C(41)-C(42)	119.49(18)
C(37)-C(34)-C(35)	110.44(16)	C(40)-C(41)-H(41)	121.6(12)
C(34)-C(35)-H(35A)	111.6(11)	C(42)-C(41)-H(41)	118.9(12)
C(34)-C(35)-H(35B)	108.9(11)	C(41)-C(42)-C(43)	120.34(19)
H(35A)-C(35)-H(35B)	109.7(15)	C(41)-C(42)-H(42)	120.7(12)
C(34)-C(35)-H(35C)	110.6(12)	C(43)-C(42)-H(42)	118.9(12)
H(35A)-C(35)-H(35C)	107.7(15)	C(42)-C(43)-C(38)	120.66(19)
H(35B)-C(35)-H(35C)	108.3(16)	C(42)-C(43)-H(43)	120.0(11)
C(34)-C(36)-H(36A)	110.8(11)	C(38)-C(43)-H(43)	119.4(11)
C(34)-C(36)-H(36B)	108.4(11)	C(49)-C(44)-C(45)	118.73(18)
H(36A)-C(36)-H(36B)	107.8(16)	C(49)-C(44)-P(1)	120.07(15)
C(34)-C(36)-H(36C)	111.6(11)	C(45)-C(44)-P(1)	121.03(15)
H(36A)-C(36)-H(36C)	111.9(15)	C(46)-C(45)-C(44)	120.12(19)
H(36B)-C(36)-H(36C)	106.1(16)	C(46)-C(45)-H(45)	120.2(11)
C(34)-C(37)-H(37A)	110.5(12)	C(44)-C(45)-H(45)	119.6(11)
C(34)-C(37)-H(37B)	107.0(12)	C(47)-C(46)-C(45)	120.6(2)

C(47)-C(46)-H(46)	120.1(11)	C(61)-C(56)-C(57)	118.63(17)
C(45)-C(46)-H(46)	119.3(11)	C(61)-C(56)-P(2)	123.97(14)
C(46)-C(47)-C(48)	119.4(2)	C(57)-C(56)-P(2)	117.16(14)
C(46)-C(47)-H(47)	121.8(13)	C(58)-C(57)-C(56)	120.69(19)
C(48)-C(47)-H(47)	118.8(12)	C(58)-C(57)-H(57)	120.7(12)
C(49)-C(48)-C(47)	120.6(2)	C(56)-C(57)-H(57)	118.6(12)
C(49)-C(48)-H(48)	120.7(13)	C(59)-C(58)-C(57)	120.2(2)
C(47)-C(48)-H(48)	118.7(13)	C(59)-C(58)-H(58)	120.6(13)
C(48)-C(49)-C(44)	120.5(2)	C(57)-C(58)-H(58)	119.2(13)
C(48)-C(49)-H(49)	121.6(12)	C(60)-C(59)-C(58)	119.7(2)
C(44)-C(49)-H(49)	117.9(12)	C(60)-C(59)-H(59)	118.9(13)
C(51)-C(50)-C(55)	118.40(17)	C(58)-C(59)-H(59)	121.4(13)
C(51)-C(50)-P(1)	123.98(14)	C(59)-C(60)-C(61)	120.7(2)
C(55)-C(50)-P(1)	117.57(14)	C(59)-C(60)-H(60)	121.2(13)
C(52)-C(51)-C(50)	121.09(18)	C(61)-C(60)-H(60)	118.1(13)
C(52)-C(51)-H(51)	118.8(13)	C(56)-C(61)-C(60)	120.17(19)
C(50)-C(51)-H(51)	120.1(13)	C(56)-C(61)-H(61)	120.4(11)
C(53)-C(52)-C(51)	119.91(19)	C(60)-C(61)-H(61)	119.4(11)
C(53)-C(52)-H(52)	118.6(13)	C(63)-C(62)-C(67)	118.75(18)
C(51)-C(52)-H(52)	121.5(13)	C(63)-C(62)-P(2)	121.96(14)
C(54)-C(53)-C(52)	119.95(19)	C(67)-C(62)-P(2)	119.11(15)
C(54)-C(53)-H(53)	120.6(13)	C(62)-C(63)-C(64)	120.0(2)
C(52)-C(53)-H(53)	119.4(13)	C(62)-C(63)-H(63)	119.6(11)
C(53)-C(54)-C(55)	120.50(19)	C(64)-C(63)-H(63)	120.3(11)
C(53)-C(54)-H(54)	118.8(12)	C(65)-C(64)-C(63)	120.1(2)
C(55)-C(54)-H(54)	120.7(12)	C(65)-C(64)-H(64)	120.8(13)
C(54)-C(55)-C(50)	120.10(18)	C(63)-C(64)-H(64)	119.2(13)
C(54)-C(55)-H(55)	122.7(12)	C(66)-C(65)-C(64)	120.3(2)
C(50)-C(55)-H(55)	117.2(12)	C(66)-C(65)-H(65)	119.6(14)

C(64)-C(65)-H(65)	120.1(14)
C(65)-C(66)-C(67)	119.8(2)
C(65)-C(66)-H(66)	122.3(12)
C(67)-C(66)-H(66)	117.9(12)
C(66)-C(67)-C(62)	120.8(2)
C(66)-C(67)-H(67)	119.9(13)
C(62)-C(67)-H(67)	119.3(13)
C(69)-C(68)-C(73)	118.63(17)
C(69)-C(68)-P(2)	118.84(14)
C(73)-C(68)-P(2)	122.50(15)
C(70)-C(69)-C(68)	120.36(19)
C(70)-C(69)-H(69)	117.9(12)
C(68)-C(69)-H(69)	121.7(12)
C(69)-C(70)-C(71)	120.3(2)
C(69)-C(70)-H(70)	121.7(13)
C(71)-C(70)-H(70)	118.0(13)
C(72)-C(71)-C(70)	120.2(2)
C(72)-C(71)-H(71)	120.6(13)
C(70)-C(71)-H(71)	119.2(13)
C(71)-C(72)-C(73)	119.92(19)
C(71)-C(72)-H(72)	122.0(12)
C(73)-C(72)-H(72)	118.0(13)
C(72)-C(73)-C(68)	120.56(19)
C(72)-C(73)-H(73)	118.9(11)
C(68)-C(73)-H(73)	120.5(11)

Table S27. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	123(1)	139(1)	84(1)	-7(1)	19(1)	2(1)
P(1)	164(2)	160(3)	97(2)	-5(2)	6(2)	14(2)
P(2)	133(2)	147(2)	125(2)	-12(2)	26(2)	3(2)
O(1)	175(6)	160(7)	142(6)	-5(5)	73(5)	-3(6)
O(2)	121(6)	171(7)	107(5)	0(5)	22(5)	-4(5)
O(3)	185(7)	251(8)	160(7)	-56(6)	9(6)	-17(6)
N(1)	114(8)	131(8)	107(7)	7(5)	29(6)	18(6)
C(1)	129(9)	187(10)	124(8)	28(7)	18(7)	34(7)
C(2)	150(10)	224(11)	113(8)	15(7)	32(7)	44(8)
C(3)	139(10)	286(12)	128(9)	58(8)	38(8)	28(8)
C(4)	141(9)	239(11)	155(9)	56(7)	12(7)	-3(8)
C(5)	146(10)	194(11)	134(8)	11(7)	20(7)	-9(8)
C(6)	135(9)	185(10)	116(8)	14(7)	26(7)	-3(7)
C(7)	135(9)	137(9)	129(8)	14(6)	47(7)	15(7)
C(8)	147(10)	155(10)	148(9)	28(7)	53(7)	-34(7)
C(9)	156(10)	146(10)	127(8)	-11(7)	22(7)	8(7)
C(10)	162(10)	164(10)	94(8)	6(7)	43(7)	-3(7)
C(11)	127(9)	122(9)	112(8)	22(6)	40(7)	36(7)
C(12)	126(8)	116(8)	107(7)	-10(7)	45(6)	-3(8)
C(13)	125(9)	128(9)	131(8)	-14(6)	14(7)	-2(7)
C(14)	173(10)	127(9)	105(8)	-4(6)	29(7)	-4(7)
C(15)	179(10)	161(10)	137(9)	-2(7)	71(8)	-33(8)
C(16)	130(9)	162(10)	127(8)	-14(6)	26(7)	-9(7)
C(17)	147(9)	102(9)	118(7)	-10(7)	21(6)	10(7)

C(18)	235(10)	228(11)	133(8)	6(8)	79(7)	64(9)
C(19)	358(14)	260(12)	203(11)	-85(9)	81(10)	3(10)
C(20)	341(14)	288(13)	210(11)	37(9)	128(10)	119(10)
C(21)	348(14)	295(13)	152(10)	14(8)	100(9)	75(10)
C(22)	197(10)	250(11)	168(9)	80(8)	17(8)	-47(8)
C(23)	286(13)	282(13)	220(11)	86(9)	-9(9)	-41(10)
C(24)	252(12)	352(14)	242(11)	106(10)	15(10)	-82(10)
C(25)	349(14)	229(13)	232(11)	63(9)	38(10)	-91(10)
C(26)	171(10)	205(10)	142(8)	-15(7)	20(7)	-63(8)
C(27)	313(13)	415(15)	217(11)	-47(10)	42(10)	-190(11)
C(28)	280(13)	226(12)	257(11)	-66(9)	26(10)	-59(10)
C(29)	207(12)	294(13)	275(11)	-10(9)	-55(10)	-30(10)
C(30)	194(10)	185(10)	109(8)	19(7)	18(7)	-22(8)
C(31)	253(12)	216(11)	194(10)	58(8)	5(9)	-39(9)
C(32)	226(12)	267(12)	140(9)	11(8)	25(8)	-11(9)
C(33)	224(11)	220(11)	138(9)	27(8)	1(8)	3(9)
C(34)	122(9)	220(11)	148(8)	-7(7)	35(7)	-16(7)
C(35)	140(11)	258(12)	218(10)	-14(8)	24(9)	-43(8)
C(36)	147(10)	316(14)	211(10)	5(8)	55(8)	-19(8)
C(37)	155(11)	261(12)	176(10)	-21(8)	41(9)	22(8)
C(38)	204(10)	154(10)	108(8)	0(7)	11(7)	64(8)
C(39)	194(10)	191(10)	139(9)	-5(7)	4(8)	47(8)
C(40)	245(11)	244(11)	165(9)	19(8)	61(8)	40(9)
C(41)	329(12)	255(12)	106(9)	4(7)	31(8)	59(9)
C(42)	310(12)	229(11)	144(9)	-41(8)	-27(9)	-17(9)
C(43)	259(12)	185(11)	148(9)	2(7)	22(8)	-19(8)
C(44)	158(10)	252(11)	87(8)	1(7)	-2(7)	29(8)
C(45)	181(10)	243(11)	132(9)	-32(7)	6(8)	34(8)
C(46)	213(11)	326(13)	159(9)	-25(8)	2(8)	-31(9)

C(47)	134(11)	461(15)	213(10)	17(9)	20(9)	21(10)
C(48)	232(12)	302(13)	280(11)	18(9)	38(9)	112(10)
C(49)	241(11)	262(12)	177(9)	17(8)	25(8)	26(9)
C(50)	144(9)	167(10)	152(8)	-22(7)	19(7)	26(7)
C(51)	225(11)	215(11)	148(9)	-7(7)	5(8)	13(8)
C(52)	250(11)	180(11)	254(10)	12(8)	13(9)	-17(8)
C(53)	271(12)	220(12)	287(11)	-76(9)	-48(9)	-19(9)
C(54)	264(12)	294(12)	167(10)	-75(8)	-40(9)	52(9)
C(55)	210(11)	211(11)	154(9)	-6(8)	10(8)	45(8)
C(56)	192(10)	134(10)	164(9)	-9(7)	60(8)	2(7)
C(57)	213(11)	234(12)	257(10)	-77(8)	28(8)	38(9)
C(58)	309(13)	319(13)	258(11)	-121(9)	-13(10)	24(10)
C(59)	389(14)	268(13)	227(11)	-89(9)	92(10)	61(10)
C(60)	257(12)	304(13)	287(11)	-39(9)	110(10)	77(10)
C(61)	208(10)	215(12)	209(9)	-21(8)	32(8)	27(8)
C(62)	208(10)	159(11)	128(8)	-15(6)	2(7)	-49(7)
C(63)	244(11)	178(10)	197(10)	-64(8)	52(8)	-47(8)
C(64)	376(14)	283(13)	219(11)	-86(8)	131(10)	-159(10)
C(65)	475(15)	263(13)	187(10)	39(9)	-1(10)	-175(11)
C(66)	353(13)	209(12)	295(11)	49(9)	-71(10)	-36(10)
C(67)	207(11)	206(11)	275(11)	14(8)	12(9)	-15(8)
C(68)	131(9)	153(10)	182(9)	-40(7)	20(7)	28(7)
C(69)	193(11)	189(11)	232(10)	-3(8)	37(9)	30(8)
C(70)	173(11)	230(12)	393(13)	-24(9)	64(10)	-22(9)
C(71)	161(11)	298(13)	365(12)	-79(9)	-35(10)	1(9)
C(72)	221(11)	271(12)	217(10)	-31(8)	-37(9)	57(9)
C(73)	175(10)	188(11)	199(10)	-24(8)	40(8)	20(8)

Table S28. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **9**.

	x	y	z	U_{iso}
H(3)	11147(13)	4630(8)	989(8)	13(5)
H(5)	10779(13)	5327(9)	2550(8)	12(5)
H(8)	11695(13)	4809(8)	3307(7)	8(5)
H(10)	10594(13)	4090(8)	4699(8)	9(5)
H(13)	10226(14)	3128(8)	4863(7)	7(4)
H(15)	7360(13)	2807(8)	5164(7)	9(5)
H(19A)	9520(15)	2778(10)	574(9)	30(6)
H(19B)	8945(18)	3438(12)	644(11)	52(7)
H(19C)	9193(16)	2936(10)	1171(10)	32(6)
H(20A)	11343(14)	2540(10)	1064(9)	27(6)
H(20B)	11041(15)	2762(10)	1694(9)	28(6)
H(20C)	11976(16)	3106(10)	1439(9)	28(6)
H(21A)	11621(16)	3813(10)	535(9)	28(6)
H(21B)	10450(14)	3945(9)	242(8)	18(5)
H(21C)	10946(16)	3270(10)	205(9)	32(6)
H(23A)	10733(16)	5616(11)	636(9)	33(6)
H(23B)	10834(16)	6350(11)	809(9)	32(6)
H(23C)	9962(16)	5948(10)	974(9)	25(6)
H(24A)	12903(16)	5609(10)	1813(9)	31(6)
H(24B)	12702(14)	6121(10)	1307(8)	19(5)
H(24C)	12553(16)	5371(10)	1184(9)	31(6)
H(25A)	10498(17)	6289(10)	2056(9)	29(6)
H(25B)	11412(14)	6666(10)	1835(8)	22(5)
H(25C)	11648(15)	6204(10)	2352(9)	28(6)
H(27A)	13261(15)	4967(10)	4014(9)	26(6)

H(27B)	13385(16)	5479(10)	4524(9)	32(6)
H(27C)	12476(16)	5602(11)	3991(10)	33(6)
H(28A)	12060(17)	5526(11)	5176(10)	39(6)
H(28B)	11110(15)	5076(10)	5123(9)	27(6)
H(28C)	11167(16)	5635(11)	4655(9)	34(6)
H(29A)	13155(16)	4122(11)	4709(9)	34(6)
H(29B)	12324(15)	4125(10)	5147(9)	25(6)
H(29C)	13282(16)	4611(10)	5215(9)	30(6)
H(31A)	9153(16)	1626(10)	5402(10)	33(6)
H(31B)	8182(16)	1871(9)	5643(8)	21(6)
H(31C)	9138(14)	1657(9)	6087(9)	23(5)
H(32A)	9188(15)	2753(9)	6585(9)	26(6)
H(32B)	8187(15)	2932(9)	6171(8)	14(5)
H(32C)	9182(13)	3365(10)	6231(8)	15(5)
H(33A)	10748(15)	2287(10)	5531(9)	25(6)
H(33B)	10731(15)	2345(10)	6192(9)	31(6)
H(33C)	10789(13)	2961(9)	5811(7)	11(5)
H(35A)	6088(14)	2781(8)	3369(8)	16(5)
H(35B)	5028(15)	2845(9)	3624(8)	18(5)
H(35C)	5845(15)	2338(11)	3905(9)	32(6)
H(36A)	5631(14)	2781(10)	4868(8)	22(5)
H(36B)	4937(16)	3380(10)	4623(8)	27(5)
H(36C)	5989(14)	3511(9)	5062(8)	19(5)
H(37A)	6176(15)	4260(10)	4237(9)	26(6)
H(37B)	5245(16)	3981(10)	3831(9)	29(6)
H(37C)	6320(14)	4023(8)	3602(8)	14(5)
H(39)	8911(13)	4811(8)	1495(8)	12(5)
H(40)	8803(14)	4864(9)	474(8)	17(5)
H(41)	7379(15)	4397(9)	-136(9)	24(5)

H(42)	6113(15)	3902(9)	295(9)	24(5)
H(43)	6258(13)	3834(9)	1302(8)	10(5)
H(45)	6122(13)	3258(9)	2352(7)	11(5)
H(46)	4351(14)	3225(9)	2368(8)	12(5)
H(47)	3493(15)	4181(9)	2440(8)	16(5)
H(48)	4356(15)	5102(10)	2527(8)	23(6)
H(49)	6139(14)	5145(9)	2521(8)	18(5)
H(51)	7824(15)	5544(9)	1880(9)	21(5)
H(52)	8319(15)	6519(10)	2289(9)	27(6)
H(53)	8856(14)	6584(10)	3290(8)	24(5)
H(54)	8880(15)	5710(9)	3894(9)	26(6)
H(55)	8354(14)	4722(9)	3461(8)	18(5)
H(57)	8366(15)	1862(9)	2045(9)	23(6)
H(58)	8555(17)	1199(10)	1254(10)	39(7)
H(59)	10236(15)	873(10)	1146(9)	30(6)
H(60)	11641(16)	1206(10)	1815(9)	30(6)
H(61)	11438(14)	1843(9)	2598(8)	20(5)
H(63)	7797(14)	2210(9)	3622(8)	11(5)
H(64)	7332(16)	1471(9)	4269(9)	25(6)
H(65)	8303(16)	557(11)	4492(10)	40(7)
H(66)	9750(14)	396(9)	4020(8)	17(5)
H(67)	10178(14)	1139(9)	3389(8)	17(5)
H(69)	11470(14)	3050(9)	2860(9)	19(5)
H(70)	13076(16)	3242(10)	3399(9)	27(6)
H(71)	13510(16)	2827(10)	4322(9)	31(6)
H(72)	12318(15)	2225(10)	4751(9)	28(6)
H(73)	10694(13)	2077(8)	4231(7)	8(5)
H(1A)	7760(20)	2888(13)	1858(11)	59(9)

$(ONO^{tBu})Ir(PPh_3)_2Cl$, 10

Crystals were mounted on a glass fiber using Paratone oil, then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S29. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **10**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	7914(1)	555(1)	6344(1)	10(1)
Cl(1)	8808(1)	-731(1)	6447(1)	14(1)
P(1)	6962(1)	-673(1)	6211(1)	12(1)
P(2)	8844(1)	1825(1)	6492(1)	12(1)
O(1)	7710(1)	354(1)	5675(1)	13(1)
O(2)	8118(1)	710(1)	7014(1)	13(1)
N(1)	7173(1)	1673(1)	6242(1)	11(1)
C(1)	7666(1)	1164(1)	5421(1)	12(1)
C(2)	7826(1)	1062(1)	5007(1)	13(1)
C(3)	7919(1)	1942(1)	4791(1)	15(1)
C(4)	7829(1)	2923(1)	4944(1)	14(1)
C(5)	7564(1)	2986(1)	5304(1)	13(1)
C(6)	7458(1)	2123(1)	5541(1)	12(1)
C(7)	7059(1)	2266(1)	5875(1)	12(1)

C(8)	6532(1)	3019(1)	5794(1)	13(1)
C(9)	6144(1)	3226(1)	6091(1)	14(1)
C(10)	6299(1)	2631(1)	6469(1)	14(1)
C(11)	6792(1)	1834(1)	6538(1)	12(1)
C(12)	6897(1)	1202(1)	6942(1)	12(1)
C(13)	6304(1)	1099(1)	7114(1)	14(1)
C(14)	6362(1)	653(1)	7517(1)	15(1)
C(15)	7061(1)	391(1)	7774(1)	16(1)
C(16)	7664(1)	476(1)	7631(1)	13(1)
C(17)	7568(1)	792(1)	7182(1)	12(1)
C(18)	7858(1)	5(1)	4801(1)	15(1)
C(19)	8453(1)	-673(1)	5089(1)	18(1)
C(20)	7991(1)	82(1)	4346(1)	21(1)
C(21)	7124(1)	-511(1)	4733(1)	17(1)
C(22)	7978(1)	3866(1)	4699(1)	17(1)
C(23)	8650(1)	3714(2)	4546(1)	32(1)
C(24)	7337(1)	4057(2)	4296(1)	33(1)
C(25)	8106(1)	4803(1)	4996(1)	33(1)
C(26)	5580(1)	4071(1)	6016(1)	17(1)
C(27)	5439(1)	4550(1)	5558(1)	26(1)
C(28)	5849(1)	4894(1)	6367(1)	26(1)
C(29)	4866(1)	3640(1)	6058(1)	24(1)
C(30)	5716(1)	449(1)	7694(1)	20(1)
C(31)	5012(1)	820(2)	7378(1)	26(1)
C(32)	5822(1)	998(2)	8135(1)	39(1)
C(33)	5651(1)	-698(2)	7755(1)	41(1)
C(34)	8425(1)	324(1)	7950(1)	15(1)
C(35)	8832(1)	1330(1)	7981(1)	19(1)
C(36)	8400(1)	63(2)	8418(1)	23(1)

C(37)	8856(1)	-516(1)	7806(1)	19(1)
C(38)	6898(1)	-1527(1)	6653(1)	14(1)
C(39)	7511(1)	-1704(1)	7002(1)	20(1)
C(40)	7501(1)	-2448(2)	7317(1)	29(1)
C(41)	6880(1)	-2984(2)	7291(1)	27(1)
C(42)	6266(1)	-2809(1)	6943(1)	24(1)
C(43)	6278(1)	-2100(1)	6621(1)	19(1)
C(44)	6912(1)	-1628(1)	5777(1)	14(1)
C(45)	7526(1)	-2101(1)	5730(1)	19(1)
C(46)	7472(1)	-2873(1)	5420(1)	23(1)
C(47)	6804(1)	-3187(1)	5161(1)	24(1)
C(48)	6191(1)	-2742(1)	5213(1)	23(1)
C(49)	6240(1)	-1963(1)	5518(1)	19(1)
C(50)	6083(1)	-59(1)	6000(1)	14(1)
C(51)	5947(1)	432(1)	5591(1)	16(1)
C(52)	5300(1)	932(1)	5412(1)	18(1)
C(53)	4782(1)	949(1)	5636(1)	21(1)
C(54)	4912(1)	469(1)	6041(1)	20(1)
C(55)	5561(1)	-32(1)	6223(1)	17(1)
C(56)	9519(1)	1772(1)	7037(1)	15(1)
C(57)	9855(1)	857(1)	7197(1)	18(1)
C(58)	10419(1)	834(1)	7586(1)	22(1)
C(59)	10650(1)	1719(1)	7821(1)	22(1)
C(60)	10321(1)	2626(1)	7666(1)	19(1)
C(61)	9760(1)	2658(1)	7276(1)	17(1)
C(62)	9446(1)	1908(1)	6143(1)	15(1)
C(63)	9401(1)	1209(1)	5808(1)	17(1)
C(64)	9879(1)	1266(1)	5552(1)	23(1)
C(65)	10403(1)	2008(2)	5632(1)	28(1)

C(66)	10463(1)	2698(2)	5973(1)	28(1)
C(67)	9990(1)	2645(1)	6229(1)	22(1)
C(68)	8487(1)	3111(1)	6504(1)	14(1)
C(69)	8556(1)	3875(1)	6218(1)	18(1)
C(70)	8268(1)	4837(1)	6245(1)	22(1)
C(71)	7909(1)	5034(1)	6558(1)	22(1)
C(72)	7844(1)	4274(1)	6848(1)	20(1)
C(73)	8130(1)	3321(1)	6823(1)	16(1)
C(81)	8975(1)	5042(2)	8395(1)	36(1)
Cl(2)	9130(1)	3954(1)	8111(1)	32(1)
Cl(3)	8150(1)	5605(1)	8120(1)	61(1)
C(82)	7220(1)	3122(2)	7834(1)	27(1)
Cl(4)	6429(1)	3844(1)	7657(1)	52(1)
Cl(5)	7499(1)	2970(1)	8411(1)	39(1)
C(83)	6002(1)	3133(1)	9423(1)	25(1)
Cl(6)	6068(1)	3247(1)	8883(1)	38(1)
Cl(7)	5502(1)	2050(1)	9484(1)	36(1)
C(84)	173(2)	2609(2)	9044(1)	45(1)
Cl(8)	482(1)	1478(1)	9322(1)	66(1)
Cl(9)	-253(1)	3398(1)	9337(1)	38(1)
C(85)	7267(2)	7481(2)	8574(1)	51(1)
Cl(10)	6505(1)	6717(1)	8452(1)	79(1)
Cl(11)	7439(1)	8095(1)	9078(1)	95(1)

Table S30. Selected bond lengths [Å] and angles [°] for **10**.

Ir(1)-N(1)	2.0194(13)	N(1)-Ir(1)-O(2)	90.61(4)
Ir(1)-O(2)	2.0459(10)	N(1)-Ir(1)-O(1)	90.67(4)
Ir(1)-O(1)	2.0511(10)	O(2)-Ir(1)-O(1)	178.30(4)
Ir(1)-Cl(1)	2.3802(4)	N(1)-Ir(1)-Cl(1)	177.91(4)
Ir(1)-P(1)	2.4010(4)	O(2)-Ir(1)-Cl(1)	90.66(3)
Ir(1)-P(2)	2.4082(4)	O(1)-Ir(1)-Cl(1)	88.10(3)
		N(1)-Ir(1)-P(1)	89.30(4)
		O(2)-Ir(1)-P(1)	99.21(3)
		O(1)-Ir(1)-P(1)	79.68(3)
		Cl(1)-Ir(1)-P(1)	92.135(13)
		N(1)-Ir(1)-P(2)	89.02(4)
		O(2)-Ir(1)-P(2)	79.46(3)
		O(1)-Ir(1)-P(2)	101.69(3)
		Cl(1)-Ir(1)-P(2)	89.581(13)
		P(1)-Ir(1)-P(2)	177.844(13)

Table S31. Bond lengths [Å] and angles [°] for **10.**

Ir(1)-N(1)	2.0194(13)	C(9)-C(10)	1.387(2)
Ir(1)-O(2)	2.0459(10)	C(9)-C(26)	1.531(2)
Ir(1)-O(1)	2.0511(10)	C(10)-C(11)	1.394(2)
Ir(1)-Cl(1)	2.3802(4)	C(11)-C(12)	1.486(2)
Ir(1)-P(1)	2.4010(4)	C(12)-C(13)	1.413(2)
Ir(1)-P(2)	2.4082(4)	C(12)-C(17)	1.411(2)
P(1)-C(38)	1.8235(16)	C(13)-C(14)	1.374(2)
P(1)-C(50)	1.8312(16)	C(14)-C(15)	1.410(2)
P(1)-C(44)	1.8422(16)	C(14)-C(30)	1.534(2)
P(2)-C(62)	1.8237(15)	C(15)-C(16)	1.376(2)
P(2)-C(68)	1.8366(16)	C(16)-C(17)	1.437(2)
P(2)-C(56)	1.8399(15)	C(16)-C(34)	1.544(2)
O(1)-C(1)	1.3239(18)	C(18)-C(20)	1.533(2)
O(2)-C(17)	1.3248(18)	C(18)-C(19)	1.536(2)
N(1)-C(11)	1.3636(19)	C(18)-C(21)	1.536(2)
N(1)-C(7)	1.3633(19)	C(22)-C(23)	1.527(2)
C(1)-C(6)	1.413(2)	C(22)-C(24)	1.524(2)
C(1)-C(2)	1.432(2)	C(22)-C(25)	1.528(2)
C(2)-C(3)	1.384(2)	C(26)-C(27)	1.530(2)
C(2)-C(18)	1.547(2)	C(26)-C(28)	1.532(2)
C(3)-C(4)	1.409(2)	C(26)-C(29)	1.538(2)
C(4)-C(5)	1.377(2)	C(30)-C(31)	1.525(2)
C(4)-C(22)	1.534(2)	C(30)-C(32)	1.530(3)
C(5)-C(6)	1.409(2)	C(30)-C(33)	1.535(3)
C(6)-C(7)	1.487(2)	C(34)-C(37)	1.533(2)
C(7)-C(8)	1.395(2)	C(34)-C(35)	1.532(2)
C(8)-C(9)	1.388(2)	C(34)-C(36)	1.531(2)

C(38)-C(39)	1.390(2)	C(66)-C(67)	1.386(2)
C(38)-C(43)	1.399(2)	C(68)-C(69)	1.385(2)
C(39)-C(40)	1.401(2)	C(68)-C(73)	1.401(2)
C(40)-C(41)	1.378(3)	C(69)-C(70)	1.397(2)
C(41)-C(42)	1.388(3)	C(70)-C(71)	1.387(3)
C(42)-C(43)	1.386(2)	C(71)-C(72)	1.386(3)
C(44)-C(45)	1.389(2)	C(72)-C(73)	1.386(2)
C(44)-C(49)	1.399(2)	C(81)-Cl(3)	1.753(2)
C(45)-C(46)	1.395(2)	C(81)-Cl(2)	1.762(2)
C(46)-C(47)	1.384(3)	C(82)-Cl(4)	1.755(2)
C(47)-C(48)	1.376(3)	C(82)-Cl(5)	1.7556(19)
C(48)-C(49)	1.392(2)	C(83)-Cl(6)	1.7500(19)
C(50)-C(55)	1.390(2)	C(83)-Cl(7)	1.7677(19)
C(50)-C(51)	1.399(2)	C(84)-Cl(8)	1.748(2)
C(51)-C(52)	1.386(2)	C(84)-Cl(9)	1.750(2)
C(52)-C(53)	1.384(2)	C(85)-Cl(11)	1.730(3)
C(53)-C(54)	1.383(2)	C(85)-Cl(10)	1.739(3)
C(54)-C(55)	1.392(2)		
C(56)-C(57)	1.396(2)	N(1)-Ir(1)-O(2)	90.61(4)
C(56)-C(61)	1.397(2)	N(1)-Ir(1)-O(1)	90.67(4)
C(57)-C(58)	1.391(2)	O(2)-Ir(1)-O(1)	178.30(4)
C(58)-C(59)	1.387(2)	N(1)-Ir(1)-Cl(1)	177.91(4)
C(59)-C(60)	1.379(3)	O(2)-Ir(1)-Cl(1)	90.66(3)
C(60)-C(61)	1.389(2)	O(1)-Ir(1)-Cl(1)	88.10(3)
C(62)-C(63)	1.388(2)	N(1)-Ir(1)-P(1)	89.30(4)
C(62)-C(67)	1.403(2)	O(2)-Ir(1)-P(1)	99.21(3)
C(63)-C(64)	1.393(2)	O(1)-Ir(1)-P(1)	79.68(3)
C(64)-C(65)	1.381(3)	Cl(1)-Ir(1)-P(1)	92.135(13)
C(65)-C(66)	1.389(3)	N(1)-Ir(1)-P(2)	89.02(4)

O(2)-Ir(1)-P(2)	79.46(3)	C(5)-C(4)-C(22)	122.30(14)
O(1)-Ir(1)-P(2)	101.69(3)	C(3)-C(4)-C(22)	120.82(13)
Cl(1)-Ir(1)-P(2)	89.581(13)	C(4)-C(5)-C(6)	122.29(14)
P(1)-Ir(1)-P(2)	177.844(13)	C(1)-C(6)-C(5)	119.03(13)
C(38)-P(1)-C(50)	106.95(7)	C(1)-C(6)-C(7)	123.39(13)
C(38)-P(1)-C(44)	98.33(7)	C(5)-C(6)-C(7)	117.27(13)
C(50)-P(1)-C(44)	100.76(7)	N(1)-C(7)-C(8)	119.71(13)
C(38)-P(1)-Ir(1)	120.00(5)	N(1)-C(7)-C(6)	122.68(13)
C(50)-P(1)-Ir(1)	110.77(5)	C(8)-C(7)-C(6)	117.56(13)
C(44)-P(1)-Ir(1)	117.71(5)	C(9)-C(8)-C(7)	121.81(14)
C(62)-P(2)-C(68)	105.54(7)	C(10)-C(9)-C(8)	116.31(14)
C(62)-P(2)-C(56)	99.14(7)	C(10)-C(9)-C(26)	121.02(13)
C(68)-P(2)-C(56)	100.82(7)	C(8)-C(9)-C(26)	122.66(13)
C(62)-P(2)-Ir(1)	119.89(5)	C(9)-C(10)-C(11)	122.12(13)
C(68)-P(2)-Ir(1)	112.33(5)	N(1)-C(11)-C(10)	119.45(13)
C(56)-P(2)-Ir(1)	116.65(5)	N(1)-C(11)-C(12)	122.01(13)
C(1)-O(1)-Ir(1)	118.67(9)	C(10)-C(11)-C(12)	118.52(13)
C(17)-O(2)-Ir(1)	118.75(9)	C(13)-C(12)-C(17)	118.89(13)
C(11)-N(1)-C(7)	120.39(13)	C(13)-C(12)-C(11)	117.09(13)
C(11)-N(1)-Ir(1)	120.34(10)	C(17)-C(12)-C(11)	123.69(13)
C(7)-N(1)-Ir(1)	119.27(10)	C(14)-C(13)-C(12)	122.47(14)
O(1)-C(1)-C(6)	122.26(13)	C(13)-C(14)-C(15)	116.65(14)
O(1)-C(1)-C(2)	118.95(13)	C(13)-C(14)-C(30)	123.58(14)
C(6)-C(1)-C(2)	118.78(13)	C(15)-C(14)-C(30)	119.77(13)
C(3)-C(2)-C(1)	117.63(14)	C(16)-C(15)-C(14)	123.94(14)
C(3)-C(2)-C(18)	121.47(13)	C(15)-C(16)-C(17)	117.72(13)
C(1)-C(2)-C(18)	120.84(13)	C(15)-C(16)-C(34)	121.32(13)
C(2)-C(3)-C(4)	123.68(14)	C(17)-C(16)-C(34)	120.77(13)
C(5)-C(4)-C(3)	116.77(14)	O(2)-C(17)-C(12)	122.73(13)

O(2)-C(17)-C(16)	118.52(13)	C(37)-C(34)-C(16)	113.65(13)
C(12)-C(17)-C(16)	118.73(13)	C(35)-C(34)-C(16)	107.89(13)
C(20)-C(18)-C(19)	107.08(13)	C(36)-C(34)-C(16)	111.69(13)
C(20)-C(18)-C(21)	107.20(13)	C(39)-C(38)-C(43)	119.27(15)
C(19)-C(18)-C(21)	109.54(13)	C(39)-C(38)-P(1)	118.65(12)
C(20)-C(18)-C(2)	111.78(13)	C(43)-C(38)-P(1)	121.58(12)
C(19)-C(18)-C(2)	112.96(12)	C(38)-C(39)-C(40)	119.87(16)
C(21)-C(18)-C(2)	108.12(12)	C(41)-C(40)-C(39)	120.35(17)
C(23)-C(22)-C(24)	108.89(15)	C(40)-C(41)-C(42)	119.95(16)
C(23)-C(22)-C(25)	107.24(16)	C(43)-C(42)-C(41)	120.12(17)
C(24)-C(22)-C(25)	109.24(16)	C(42)-C(43)-C(38)	120.36(15)
C(23)-C(22)-C(4)	110.68(14)	C(45)-C(44)-C(49)	118.66(15)
C(24)-C(22)-C(4)	109.14(14)	C(45)-C(44)-P(1)	121.50(12)
C(25)-C(22)-C(4)	111.59(13)	C(49)-C(44)-P(1)	119.52(12)
C(27)-C(26)-C(28)	108.89(15)	C(44)-C(45)-C(46)	120.53(15)
C(27)-C(26)-C(9)	111.95(13)	C(47)-C(46)-C(45)	120.22(17)
C(28)-C(26)-C(9)	108.88(13)	C(48)-C(47)-C(46)	119.73(16)
C(27)-C(26)-C(29)	108.19(14)	C(47)-C(48)-C(49)	120.49(16)
C(28)-C(26)-C(29)	109.11(14)	C(48)-C(49)-C(44)	120.33(16)
C(9)-C(26)-C(29)	109.77(14)	C(55)-C(50)-C(51)	118.83(14)
C(31)-C(30)-C(14)	112.15(13)	C(55)-C(50)-P(1)	124.34(12)
C(31)-C(30)-C(32)	107.80(15)	C(51)-C(50)-P(1)	116.81(11)
C(14)-C(30)-C(32)	109.72(14)	C(52)-C(51)-C(50)	120.42(15)
C(31)-C(30)-C(33)	107.98(16)	C(53)-C(52)-C(51)	120.30(15)
C(14)-C(30)-C(33)	108.95(14)	C(54)-C(53)-C(52)	119.77(15)
C(32)-C(30)-C(33)	110.21(17)	C(53)-C(54)-C(55)	120.25(15)
C(37)-C(34)-C(35)	109.34(13)	C(50)-C(55)-C(54)	120.42(15)
C(37)-C(34)-C(36)	107.15(13)	C(57)-C(56)-C(61)	118.52(14)
C(35)-C(34)-C(36)	106.91(13)	C(57)-C(56)-P(2)	120.36(12)

C(61)-C(56)-P(2)	120.80(12)
C(58)-C(57)-C(56)	120.44(16)
C(59)-C(58)-C(57)	120.35(17)
C(60)-C(59)-C(58)	119.63(15)
C(59)-C(60)-C(61)	120.42(16)
C(60)-C(61)-C(56)	120.65(16)
C(63)-C(62)-C(67)	119.15(14)
C(63)-C(62)-P(2)	120.65(12)
C(67)-C(62)-P(2)	120.08(12)
C(62)-C(63)-C(64)	119.88(16)
C(65)-C(64)-C(63)	120.69(16)
C(66)-C(65)-C(64)	119.92(16)
C(65)-C(66)-C(67)	119.72(17)
C(66)-C(67)-C(62)	120.60(16)
C(69)-C(68)-C(73)	118.95(15)
C(69)-C(68)-P(2)	123.42(12)
C(73)-C(68)-P(2)	117.63(12)
C(68)-C(69)-C(70)	120.46(15)
C(71)-C(70)-C(69)	120.17(16)
C(72)-C(71)-C(70)	119.62(16)
C(71)-C(72)-C(73)	120.33(16)
C(72)-C(73)-C(68)	120.46(15)
Cl(3)-C(81)-Cl(2)	110.95(12)
Cl(4)-C(82)-Cl(5)	111.97(11)
Cl(6)-C(83)-Cl(7)	111.76(10)
Cl(8)-C(84)-Cl(9)	112.79(13)
Cl(11)-C(85)-Cl(10)	113.77(16)

Table S32. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	92(1)	116(1)	84(1)	2(1)	23(1)	11(1)
Cl(1)	132(2)	149(2)	137(1)	-1(1)	17(1)	35(1)
P(1)	111(2)	130(2)	107(1)	2(1)	23(1)	1(1)
P(2)	112(2)	141(2)	101(2)	-9(1)	32(1)	-6(1)
O(1)	150(5)	137(6)	92(4)	1(4)	33(4)	8(4)
O(2)	109(4)	193(6)	94(4)	2(4)	33(3)	14(4)
N(1)	112(5)	129(6)	87(5)	-13(4)	23(4)	-9(5)
C(1)	99(6)	144(7)	109(6)	0(5)	24(5)	3(5)
C(2)	121(6)	146(8)	110(6)	-12(5)	30(5)	17(5)
C(3)	152(7)	181(8)	116(6)	-11(5)	54(5)	-2(6)
C(4)	145(6)	162(8)	125(6)	12(5)	40(5)	10(6)
C(5)	149(6)	122(7)	125(6)	-4(5)	37(5)	17(5)
C(6)	119(6)	145(7)	99(6)	1(5)	32(5)	13(5)
C(7)	120(6)	122(7)	104(6)	-11(5)	26(5)	4(5)
C(8)	148(6)	131(7)	121(6)	17(5)	37(5)	24(5)
C(9)	138(6)	131(7)	133(6)	-13(5)	36(5)	15(5)
C(10)	144(6)	155(8)	126(6)	-13(5)	54(5)	16(5)
C(11)	107(6)	138(7)	109(6)	-16(5)	25(5)	-13(5)
C(12)	124(6)	137(7)	106(6)	-11(5)	31(5)	3(5)
C(13)	126(6)	167(8)	123(6)	-13(5)	37(5)	8(5)
C(14)	143(6)	171(8)	141(6)	-12(6)	56(5)	-15(6)
C(15)	161(6)	190(9)	125(6)	9(5)	52(5)	-7(6)
C(16)	138(6)	146(7)	109(5)	7(5)	36(4)	12(6)
C(17)	116(6)	131(7)	113(6)	-5(5)	36(5)	-8(5)

C(18)	163(7)	153(8)	126(6)	-20(5)	49(5)	13(6)
C(19)	176(7)	162(8)	196(7)	-32(6)	55(5)	27(6)
C(20)	303(9)	183(9)	178(7)	-37(6)	129(6)	-7(7)
C(21)	174(7)	155(8)	164(6)	-22(6)	35(5)	-9(6)
C(22)	218(8)	151(8)	150(6)	15(6)	75(6)	1(6)
C(23)	335(10)	247(10)	452(12)	99(9)	251(9)	23(8)
C(24)	332(11)	302(11)	288(9)	143(8)	-2(8)	-52(9)
C(25)	609(14)	181(9)	251(9)	-18(7)	224(9)	-99(9)
C(26)	165(7)	172(8)	172(7)	-2(6)	53(5)	49(6)
C(27)	286(9)	246(10)	242(8)	44(7)	89(7)	137(8)
C(28)	243(9)	221(10)	300(9)	-75(7)	44(7)	68(7)
C(29)	179(8)	270(10)	291(9)	12(7)	78(7)	61(7)
C(30)	147(6)	287(10)	172(6)	30(7)	76(5)	-10(7)
C(31)	143(7)	409(12)	239(8)	35(7)	83(6)	-1(7)
C(32)	215(9)	795(17)	209(8)	-96(10)	122(7)	-59(10)
C(33)	272(10)	383(13)	632(15)	195(11)	228(10)	-12(9)
C(34)	141(6)	202(9)	112(6)	13(5)	28(5)	12(5)
C(35)	161(7)	247(9)	151(7)	-19(6)	19(5)	-5(6)
C(36)	197(8)	346(11)	131(7)	50(7)	31(6)	22(7)
C(37)	165(7)	224(9)	174(6)	30(7)	26(5)	45(7)
C(38)	179(7)	131(8)	123(6)	-2(5)	41(5)	-5(6)
C(39)	202(8)	200(9)	179(7)	35(6)	20(6)	-36(6)
C(40)	302(10)	300(11)	215(8)	105(7)	-25(7)	-65(8)
C(41)	350(10)	260(10)	197(8)	79(7)	54(7)	-76(8)
C(42)	268(9)	231(9)	218(8)	17(7)	79(7)	-93(7)
C(43)	187(7)	206(9)	177(7)	7(6)	35(6)	-43(6)
C(44)	166(7)	120(7)	130(6)	5(5)	35(5)	-5(6)
C(45)	175(7)	174(8)	206(7)	-23(6)	34(6)	-1(6)
C(46)	235(8)	172(9)	276(8)	-40(7)	80(7)	23(7)

C(47)	307(9)	180(9)	208(8)	-58(7)	51(7)	-4(7)
C(48)	226(8)	226(9)	203(8)	-60(7)	-3(6)	-30(7)
C(49)	172(7)	200(9)	183(7)	-38(6)	18(6)	-8(6)
C(50)	124(6)	137(8)	141(6)	-21(5)	15(5)	-13(5)
C(51)	145(6)	170(8)	157(6)	-5(6)	34(5)	0(6)
C(52)	162(7)	168(8)	192(7)	21(6)	2(6)	11(6)
C(53)	125(7)	185(8)	277(8)	-28(7)	6(6)	17(6)
C(54)	143(6)	203(9)	245(7)	-43(7)	59(5)	-8(6)
C(55)	146(7)	184(8)	161(7)	-31(6)	32(5)	-24(6)
C(56)	117(6)	198(8)	129(6)	-11(6)	35(5)	-11(6)
C(57)	158(7)	185(8)	185(7)	-24(6)	20(5)	3(6)
C(58)	178(7)	242(9)	207(7)	12(6)	-2(6)	16(6)
C(59)	155(7)	314(10)	163(7)	1(7)	-5(5)	-27(7)
C(60)	186(7)	229(9)	152(7)	-39(6)	23(6)	-48(6)
C(61)	164(7)	184(8)	149(6)	-12(6)	35(5)	-21(6)
C(62)	140(6)	185(8)	142(6)	-4(6)	51(5)	-8(6)
C(63)	153(7)	197(8)	154(6)	-12(6)	52(5)	-4(6)
C(64)	239(8)	273(10)	205(7)	-73(7)	114(6)	-35(7)
C(65)	271(9)	334(11)	305(9)	-62(8)	190(8)	-61(8)
C(66)	262(9)	310(11)	325(9)	-100(8)	178(8)	-125(8)
C(67)	224(8)	265(10)	221(8)	-88(7)	117(6)	-80(7)
C(68)	134(6)	152(8)	133(6)	-12(5)	17(5)	-6(5)
C(69)	205(8)	180(8)	149(6)	-15(6)	41(6)	-25(6)
C(70)	255(9)	170(9)	210(8)	23(6)	27(6)	-31(7)
C(71)	202(8)	168(9)	261(8)	-35(7)	9(6)	18(6)
C(72)	166(7)	212(9)	221(7)	-44(6)	54(6)	0(6)
C(73)	155(7)	165(8)	165(6)	-24(6)	41(5)	-12(6)
C(81)	300(10)	452(14)	304(10)	6(9)	63(8)	-6(9)

Cl(2)	286(2)	316(3)	375(3)	2(2)	99(2)	-42(2)
Cl(3)	535(4)	448(4)	708(4)	16(3)	-66(3)	208(3)
C(82)	242(9)	315(11)	236(8)	-18(7)	50(7)	22(8)
Cl(4)	414(3)	587(4)	497(3)	-39(3)	10(3)	242(3)
Cl(5)	431(3)	523(3)	237(2)	0(2)	140(2)	73(3)
C(83)	225(8)	243(10)	284(9)	-10(7)	61(7)	-48(7)
Cl(6)	515(3)	348(3)	357(3)	-3(2)	242(2)	69(2)
Cl(7)	301(2)	274(3)	525(3)	-7(2)	168(2)	-71(2)
C(84)	544(15)	433(14)	390(12)	66(11)	178(11)	80(12)
Cl(8)	461(4)	559(4)	1082(6)	410(4)	406(4)	244(3)
Cl(9)	370(3)	377(3)	403(3)	5(2)	112(2)	-33(2)
C(85)	483(15)	586(17)	478(14)	-29(12)	174(12)	-97(13)
Cl(10)	595(5)	1043(7)	647(5)	164(5)	30(4)	-388(5)
Cl(11)	1653(11)	591(5)	825(6)	-318(4)	721(7)	-443(6)

$(ONO^{tBu})Ir(PPh_3)_2H$, 11

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The crystal contains pentane as a solvent of crystallization. The pentane was refined without restraints except for riding hydrogens. All other hydrogens were refined without restraint with the exception of the hydride on Ir, where the position was allowed to refined but the U_{iso} was fixed at U_{iso}=0.03.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S33. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **11**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	7055(1)	9383(1)	7210(1)	12(1)
P(1)	6879(1)	10329(1)	6885(1)	15(1)
P(2)	7133(1)	8411(1)	7215(1)	13(1)
O(1)	5951(1)	9280(1)	7529(1)	15(1)
O(2)	8198(1)	9500(1)	6966(1)	15(1)
N(1)	7590(1)	9486(1)	8404(1)	12(1)
C(1)	5742(1)	9637(1)	8029(1)	14(1)
C(2)	4890(1)	9736(1)	8003(1)	15(1)
C(3)	4682(1)	10165(1)	8455(1)	16(1)
C(4)	5248(1)	10513(1)	8944(1)	15(1)
C(5)	6059(1)	10368(1)	9027(1)	14(1)
C(6)	6314(1)	9922(1)	8610(1)	13(1)
C(7)	7162(1)	9722(1)	8897(1)	12(1)
C(8)	7496(1)	9760(1)	9698(1)	14(1)
C(9)	8285(1)	9590(1)	10014(1)	13(1)
C(10)	8713(1)	9370(1)	9487(1)	13(1)
C(11)	8366(1)	9303(1)	8698(1)	12(1)
C(12)	8871(1)	9065(1)	8178(1)	13(1)
C(13)	9491(1)	8685(1)	8531(1)	14(1)
C(14)	10126(1)	8544(1)	8183(1)	15(1)
C(15)	10168(1)	8835(1)	7496(1)	17(1)

C(16)	9565(1)	9187(1)	7099(1)	15(1)
C(17)	8844(1)	9254(1)	7408(1)	13(1)
C(18)	4244(1)	9364(1)	7480(1)	19(1)
C(19)	4404(1)	8748(1)	7728(1)	22(1)
C(20)	4262(1)	9443(1)	6614(1)	23(1)
C(21)	3379(1)	9506(1)	7579(2)	29(1)
C(22)	4973(1)	11019(1)	9363(1)	17(1)
C(23)	4594(2)	11459(1)	8754(2)	32(1)
C(24)	4338(1)	10840(1)	9827(2)	27(1)
C(25)	5682(1)	11290(1)	9935(2)	28(1)
C(26)	8682(1)	9634(1)	10882(1)	16(1)
C(27)	8937(1)	9049(1)	11206(1)	25(1)
C(28)	9444(1)	10009(1)	10972(1)	22(1)
C(29)	8117(1)	9889(1)	11366(1)	24(1)
C(30)	10774(1)	8107(1)	8530(1)	20(1)
C(31)	11603(1)	8399(1)	8796(2)	29(1)
C(32)	10563(1)	7802(1)	9227(2)	25(1)
C(33)	10841(2)	7666(1)	7905(2)	35(1)
C(34)	9654(1)	9499(1)	6351(1)	19(1)
C(35)	9539(1)	10132(1)	6457(2)	23(1)
C(36)	9033(1)	9281(1)	5634(1)	22(1)
C(37)	10503(1)	9415(1)	6178(2)	29(1)
C(38)	5833(1)	10579(1)	6498(1)	17(1)
C(39)	5338(1)	10771(1)	6987(1)	19(1)
C(40)	4555(1)	10966(1)	6672(1)	24(1)
C(41)	4249(1)	10952(1)	5878(1)	27(1)
C(42)	4720(1)	10741(1)	5387(2)	28(1)
C(43)	5513(1)	10561(1)	5694(1)	23(1)
C(44)	7344(1)	10818(1)	7656(1)	16(1)

C(45)	6986(1)	11304(1)	7865(1)	20(1)
C(46)	7372(1)	11623(1)	8499(1)	24(1)
C(47)	8130(1)	11470(1)	8923(2)	29(1)
C(48)	8513(1)	10999(1)	8706(1)	28(1)
C(49)	8126(1)	10676(1)	8080(1)	20(1)
C(50)	7354(1)	10524(1)	6073(1)	20(1)
C(51)	7660(1)	11062(1)	6032(2)	26(1)
C(52)	7943(1)	11231(1)	5372(2)	33(1)
C(53)	7907(1)	10862(1)	4752(2)	30(1)
C(54)	7616(1)	10329(1)	4794(1)	27(1)
C(55)	7342(1)	10157(1)	5450(1)	22(1)
C(56)	6163(1)	8048(1)	6864(1)	15(1)
C(57)	5542(1)	8300(1)	6319(1)	20(1)
C(58)	4839(1)	8003(1)	5992(1)	26(1)
C(59)	4746(1)	7456(1)	6221(1)	26(1)
C(60)	5351(1)	7204(1)	6774(1)	26(1)
C(61)	6058(1)	7501(1)	7095(1)	21(1)
C(62)	7477(1)	8069(1)	8164(1)	15(1)
C(63)	7126(1)	8268(1)	8768(1)	18(1)
C(64)	7320(1)	8036(1)	9506(1)	24(1)
C(65)	7869(1)	7595(1)	9658(1)	26(1)
C(66)	8210(1)	7389(1)	9067(1)	25(1)
C(67)	8021(1)	7620(1)	8326(1)	19(1)
C(68)	7724(1)	8139(1)	6530(1)	14(1)
C(69)	8559(1)	8024(1)	6743(1)	18(1)
C(70)	8972(1)	7824(1)	6188(1)	22(1)
C(71)	8573(1)	7749(1)	5422(1)	23(1)
C(72)	7752(1)	7881(1)	5194(1)	23(1)
C(73)	7333(1)	8069(1)	5745(1)	19(1)

C(81)	5204(2)	7365(1)	8905(2)	61(1)
C(82)	4333(2)	7275(1)	8469(2)	64(1)
C(83)	4025(2)	6689(1)	8530(2)	51(1)
C(84)	3171(2)	6567(2)	8123(2)	77(1)
C(85)	2857(2)	6017(2)	8268(3)	106(2)

Table S34. Selected bond lengths [Å] and angles [°] for **11**.

Ir(1)-O(1)	2.0663(11)	O(1)-Ir(1)-O(2)	176.19(5)
Ir(1)-O(2)	2.0764(11)	O(1)-Ir(1)-N(1)	87.97(5)
Ir(1)-N(1)	2.1020(16)	O(2)-Ir(1)-N(1)	88.25(5)
Ir(1)-P(2)	2.3229(5)	O(1)-Ir(1)-P(2)	86.17(4)
Ir(1)-P(1)	2.3320(5)	O(2)-Ir(1)-P(2)	94.68(3)
Ir(1)-H(1)	1.70(2)	N(1)-Ir(1)-P(2)	95.82(4)
		O(1)-Ir(1)-P(1)	96.13(4)
		O(2)-Ir(1)-P(1)	83.91(3)
		N(1)-Ir(1)-P(1)	97.67(4)
		P(2)-Ir(1)-P(1)	166.384(19)
		O(1)-Ir(1)-H(1)	95.6(6)
		O(2)-Ir(1)-H(1)	88.2(6)
		N(1)-Ir(1)-H(1)	176.3(7)
		P(2)-Ir(1)-H(1)	85.7(7)
		P(1)-Ir(1)-H(1)	80.7(7)

Table S35. Bond lengths [Å] and angles [°] for **11**.

Ir(1)-O(1)	2.0663(11)	C(7)-C(8)	1.395(3)
Ir(1)-O(2)	2.0764(11)	C(8)-C(9)	1.386(2)
Ir(1)-N(1)	2.1020(16)	C(8)-H(8)	0.902(18)
Ir(1)-P(2)	2.3229(5)	C(9)-C(10)	1.388(3)
Ir(1)-P(1)	2.3320(5)	C(9)-C(26)	1.525(3)
Ir(1)-H(1)	1.70(2)	C(10)-C(11)	1.386(3)
P(1)-C(44)	1.827(2)	C(10)-H(10)	0.931(18)
P(1)-C(50)	1.831(2)	C(11)-C(12)	1.484(2)
P(1)-C(38)	1.8451(17)	C(12)-C(17)	1.410(3)
P(2)-C(62)	1.828(2)	C(12)-C(13)	1.420(2)
P(2)-C(68)	1.8314(19)	C(13)-C(14)	1.380(2)
P(2)-C(56)	1.8357(17)	C(13)-H(13)	0.925(18)
O(1)-C(1)	1.321(2)	C(14)-C(15)	1.401(3)
O(2)-C(17)	1.329(2)	C(14)-C(30)	1.536(2)
N(1)-C(7)	1.359(2)	C(15)-C(16)	1.385(3)
N(1)-C(11)	1.368(2)	C(15)-H(15)	0.969(18)
C(1)-C(6)	1.414(2)	C(16)-C(17)	1.439(2)
C(1)-C(2)	1.445(2)	C(16)-C(34)	1.538(3)
C(2)-C(3)	1.383(3)	C(18)-C(20)	1.532(3)
C(2)-C(18)	1.543(3)	C(18)-C(19)	1.540(3)
C(3)-C(4)	1.408(3)	C(18)-C(21)	1.541(3)
C(3)-H(3)	0.967(17)	C(19)-H(19A)	0.969(18)
C(4)-C(5)	1.387(2)	C(19)-H(19B)	0.93(2)
C(4)-C(22)	1.533(3)	C(19)-H(19C)	1.02(2)
C(5)-C(6)	1.408(3)	C(20)-H(20A)	0.97(2)
C(5)-H(5)	0.941(18)	C(20)-H(20B)	0.97(2)
C(6)-C(7)	1.486(2)	C(20)-H(20C)	0.952(19)

C(21)-H(21A)	0.95(2)	C(30)-C(31)	1.540(3)
C(21)-H(21B)	0.94(2)	C(31)-H(31A)	0.91(2)
C(21)-H(21C)	1.01(2)	C(31)-H(31B)	0.95(2)
C(22)-C(23)	1.534(3)	C(31)-H(31C)	0.98(2)
C(22)-C(25)	1.528(3)	C(32)-H(32A)	0.93(2)
C(22)-C(24)	1.534(3)	C(32)-H(32B)	0.96(2)
C(23)-H(23A)	0.98(2)	C(32)-H(32C)	0.92(2)
C(23)-H(23B)	0.95(3)	C(33)-H(33A)	0.99(3)
C(23)-H(23C)	0.95(2)	C(33)-H(33B)	1.00(3)
C(24)-H(24A)	0.96(2)	C(33)-H(33C)	0.98(2)
C(24)-H(24B)	1.04(2)	C(34)-C(37)	1.535(3)
C(24)-H(24C)	0.92(2)	C(34)-C(35)	1.540(3)
C(25)-H(25A)	1.01(2)	C(34)-C(36)	1.540(3)
C(25)-H(25B)	0.97(2)	C(35)-H(35A)	0.96(2)
C(25)-H(25C)	0.97(2)	C(35)-H(35B)	1.02(2)
C(26)-C(27)	1.533(3)	C(35)-H(35C)	0.93(2)
C(26)-C(29)	1.528(3)	C(36)-H(36A)	0.95(2)
C(26)-C(28)	1.544(3)	C(36)-H(36B)	1.01(2)
C(27)-H(27A)	0.93(2)	C(36)-H(36C)	0.979(18)
C(27)-H(27B)	0.97(3)	C(37)-H(37A)	0.95(2)
C(27)-H(27C)	1.00(2)	C(37)-H(37B)	0.98(2)
C(28)-H(28A)	0.95(2)	C(37)-H(37C)	0.94(2)
C(28)-H(28B)	0.92(2)	C(38)-C(39)	1.393(3)
C(28)-H(28C)	0.95(2)	C(38)-C(43)	1.393(3)
C(29)-H(29A)	0.89(2)	C(39)-C(40)	1.394(3)
C(29)-H(29B)	0.97(2)	C(39)-H(39)	0.874(19)
C(29)-H(29C)	0.96(2)	C(40)-C(41)	1.373(3)
C(30)-C(32)	1.525(3)	C(40)-H(40)	0.96(2)
C(30)-C(33)	1.539(3)	C(41)-C(42)	1.382(3)

C(41)-H(41)	0.91(2)	C(57)-H(57)	0.93(2)
C(42)-C(43)	1.395(3)	C(58)-C(59)	1.383(3)
C(42)-H(42)	0.92(2)	C(58)-H(58)	0.89(2)
C(43)-H(43)	0.952(18)	C(59)-C(60)	1.383(3)
C(44)-C(45)	1.392(3)	C(59)-H(59)	0.98(2)
C(44)-C(49)	1.406(3)	C(60)-C(61)	1.395(3)
C(45)-C(46)	1.386(3)	C(60)-H(60)	0.97(2)
C(45)-H(45)	0.915(18)	C(61)-H(61)	0.944(19)
C(46)-C(47)	1.380(3)	C(62)-C(63)	1.400(3)
C(46)-H(46)	0.94(2)	C(62)-C(67)	1.397(3)
C(47)-C(48)	1.390(3)	C(63)-C(64)	1.378(3)
C(47)-H(47)	0.94(2)	C(63)-H(63)	0.891(18)
C(48)-C(49)	1.381(3)	C(64)-C(65)	1.387(3)
C(48)-H(48)	0.977(19)	C(64)-H(64)	0.89(2)
C(49)-H(49)	0.93(2)	C(65)-C(66)	1.376(3)
C(50)-C(55)	1.394(3)	C(65)-H(65)	0.88(2)
C(50)-C(51)	1.393(3)	C(66)-C(67)	1.380(3)
C(51)-C(52)	1.399(3)	C(66)-H(66)	0.89(2)
C(51)-H(51)	0.95(2)	C(67)-H(67)	0.88(2)
C(52)-C(53)	1.386(4)	C(68)-C(69)	1.402(2)
C(52)-H(52)	0.98(2)	C(68)-C(73)	1.398(3)
C(53)-C(54)	1.371(3)	C(69)-C(70)	1.392(3)
C(53)-H(53)	0.94(2)	C(69)-H(69)	0.897(19)
C(54)-C(55)	1.387(3)	C(70)-C(71)	1.375(3)
C(54)-H(54)	0.93(2)	C(70)-H(70)	0.981(18)
C(55)-H(55)	1.02(2)	C(71)-C(72)	1.390(3)
C(56)-C(61)	1.388(3)	C(71)-H(71)	0.91(2)
C(56)-C(57)	1.391(3)	C(72)-C(73)	1.385(3)
C(57)-C(58)	1.392(3)	C(72)-H(72)	0.92(2)

C(73)-H(73)	0.959(18)	O(2)-Ir(1)-H(1)	88.2(6)
C(81)-C(82)	1.515(4)	N(1)-Ir(1)-H(1)	176.3(7)
C(81)-H(81A)	0.9800	P(2)-Ir(1)-H(1)	85.7(7)
C(81)-H(81B)	0.9800	P(1)-Ir(1)-H(1)	80.7(7)
C(81)-H(81C)	0.9800	C(44)-P(1)-C(50)	102.79(9)
C(82)-C(83)	1.503(4)	C(44)-P(1)-C(38)	106.70(9)
C(82)-H(82A)	0.9900	C(50)-P(1)-C(38)	100.04(9)
C(82)-H(82B)	0.9900	C(44)-P(1)-Ir(1)	115.25(7)
C(83)-C(84)	1.490(4)	C(50)-P(1)-Ir(1)	112.39(6)
C(83)-H(83A)	0.9900	C(38)-P(1)-Ir(1)	117.65(6)
C(83)-H(83B)	0.9900	C(62)-P(2)-C(68)	108.85(9)
C(84)-C(85)	1.457(5)	C(62)-P(2)-C(56)	100.22(8)
C(84)-H(84A)	0.9900	C(68)-P(2)-C(56)	100.51(8)
C(84)-H(84B)	0.9900	C(62)-P(2)-Ir(1)	117.18(6)
C(85)-H(85A)	0.9800	C(68)-P(2)-Ir(1)	112.98(6)
C(85)-H(85B)	0.9800	C(56)-P(2)-Ir(1)	115.19(6)
C(85)-H(85C)	0.9800	C(1)-O(1)-Ir(1)	118.91(11)
		C(17)-O(2)-Ir(1)	119.94(11)
O(1)-Ir(1)-O(2)	176.19(5)	C(7)-N(1)-C(11)	119.12(16)
O(1)-Ir(1)-N(1)	87.97(5)	C(7)-N(1)-Ir(1)	120.39(11)
O(2)-Ir(1)-N(1)	88.25(5)	C(11)-N(1)-Ir(1)	120.47(12)
O(1)-Ir(1)-P(2)	86.17(4)	O(1)-C(1)-C(6)	123.28(15)
O(2)-Ir(1)-P(2)	94.68(3)	O(1)-C(1)-C(2)	119.14(16)
N(1)-Ir(1)-P(2)	95.82(4)	C(6)-C(1)-C(2)	117.56(17)
O(1)-Ir(1)-P(1)	96.13(4)	C(3)-C(2)-C(1)	118.29(17)
O(2)-Ir(1)-P(1)	83.91(3)	C(3)-C(2)-C(18)	122.11(15)
N(1)-Ir(1)-P(1)	97.67(4)	C(1)-C(2)-C(18)	119.60(16)
P(2)-Ir(1)-P(1)	166.384(19)	C(2)-C(3)-C(4)	124.25(16)
O(1)-Ir(1)-H(1)	95.6(6)	C(2)-C(3)-H(3)	117.5(12)

C(4)-C(3)-H(3)	118.1(12)	C(14)-C(13)-H(13)	123.0(10)
C(5)-C(4)-C(3)	116.06(17)	C(12)-C(13)-H(13)	115.0(10)
C(5)-C(4)-C(22)	122.52(17)	C(13)-C(14)-C(15)	116.28(17)
C(3)-C(4)-C(22)	121.42(15)	C(13)-C(14)-C(30)	122.86(18)
C(4)-C(5)-C(6)	122.49(17)	C(15)-C(14)-C(30)	120.84(16)
C(4)-C(5)-H(5)	121.1(11)	C(16)-C(15)-C(14)	124.37(17)
C(6)-C(5)-H(5)	116.4(11)	C(16)-C(15)-H(15)	116.3(11)
C(5)-C(6)-C(1)	119.95(15)	C(14)-C(15)-H(15)	119.1(11)
C(5)-C(6)-C(7)	116.43(16)	C(15)-C(16)-C(17)	117.68(18)
C(1)-C(6)-C(7)	122.98(16)	C(15)-C(16)-C(34)	121.67(16)
N(1)-C(7)-C(8)	120.64(15)	C(17)-C(16)-C(34)	120.65(16)
N(1)-C(7)-C(6)	121.36(16)	O(2)-C(17)-C(12)	123.46(15)
C(8)-C(7)-C(6)	117.93(16)	O(2)-C(17)-C(16)	118.72(17)
C(9)-C(8)-C(7)	121.72(17)	C(12)-C(17)-C(16)	117.80(16)
C(9)-C(8)-H(8)	121.4(12)	C(20)-C(18)-C(19)	110.94(18)
C(7)-C(8)-H(8)	116.9(12)	C(20)-C(18)-C(21)	107.60(17)
C(8)-C(9)-C(10)	115.86(17)	C(19)-C(18)-C(21)	106.91(17)
C(8)-C(9)-C(26)	123.66(17)	C(20)-C(18)-C(2)	110.66(16)
C(10)-C(9)-C(26)	120.48(15)	C(19)-C(18)-C(2)	108.99(15)
C(9)-C(10)-C(11)	122.33(15)	C(21)-C(18)-C(2)	111.69(17)
C(9)-C(10)-H(10)	118.9(13)	C(18)-C(19)-H(19A)	112.8(12)
C(11)-C(10)-H(10)	118.7(13)	C(18)-C(19)-H(19B)	109.3(14)
N(1)-C(11)-C(10)	120.17(16)	H(19A)-C(19)-H(19B)	107.7(17)
N(1)-C(11)-C(12)	121.16(16)	C(18)-C(19)-H(19C)	109.9(12)
C(10)-C(11)-C(12)	118.55(14)	H(19A)-C(19)-H(19C)	111.0(17)
C(17)-C(12)-C(13)	119.24(16)	H(19B)-C(19)-H(19C)	105.9(17)
C(17)-C(12)-C(11)	123.85(15)	C(18)-C(20)-H(20A)	111.1(13)
C(13)-C(12)-C(11)	116.26(17)	C(18)-C(20)-H(20B)	111.4(14)
C(14)-C(13)-C(12)	122.06(18)	H(20A)-C(20)-H(20B)	106.0(17)

C(18)-C(20)-H(20C)	114.5(13)	H(25A)-C(25)-H(25B)	103.3(19)
H(20A)-C(20)-H(20C)	104.9(17)	C(22)-C(25)-H(25C)	113.2(14)
H(20B)-C(20)-H(20C)	108.4(17)	H(25A)-C(25)-H(25C)	109.0(17)
C(18)-C(21)-H(21A)	112.0(13)	H(25B)-C(25)-H(25C)	110.2(18)
C(18)-C(21)-H(21B)	106.8(12)	C(9)-C(26)-C(27)	109.34(17)
H(21A)-C(21)-H(21B)	109.0(18)	C(9)-C(26)-C(29)	112.67(15)
C(18)-C(21)-H(21C)	111.3(11)	C(27)-C(26)-C(29)	108.50(18)
H(21A)-C(21)-H(21C)	109.5(18)	C(9)-C(26)-C(28)	108.60(16)
H(21B)-C(21)-H(21C)	108.2(17)	C(27)-C(26)-C(28)	109.29(16)
C(23)-C(22)-C(25)	108.23(19)	C(29)-C(26)-C(28)	108.40(17)
C(23)-C(22)-C(4)	109.31(18)	C(26)-C(27)-H(27A)	108.4(14)
C(25)-C(22)-C(4)	111.94(15)	C(26)-C(27)-H(27B)	109.9(14)
C(23)-C(22)-C(24)	108.95(18)	H(27A)-C(27)-H(27B)	107(2)
C(25)-C(22)-C(24)	107.88(19)	C(26)-C(27)-H(27C)	113.5(13)
C(4)-C(22)-C(24)	110.45(16)	H(27A)-C(27)-H(27C)	109.2(19)
C(22)-C(23)-H(23A)	110.8(13)	H(27B)-C(27)-H(27C)	108.2(17)
C(22)-C(23)-H(23B)	108.8(16)	C(26)-C(28)-H(28A)	111.9(12)
H(23A)-C(23)-H(23B)	109.2(19)	C(26)-C(28)-H(28B)	109.5(13)
C(22)-C(23)-H(23C)	111.5(15)	H(28A)-C(28)-H(28B)	109.6(17)
H(23A)-C(23)-H(23C)	110(2)	C(26)-C(28)-H(28C)	109.8(12)
H(23B)-C(23)-H(23C)	106.6(19)	H(28A)-C(28)-H(28C)	109.6(18)
C(22)-C(24)-H(24A)	110.3(14)	H(28B)-C(28)-H(28C)	106.3(18)
C(22)-C(24)-H(24B)	110.8(12)	C(26)-C(29)-H(29A)	109.8(15)
H(24A)-C(24)-H(24B)	109.3(16)	C(26)-C(29)-H(29B)	109.8(11)
C(22)-C(24)-H(24C)	112.9(14)	H(29A)-C(29)-H(29B)	109.7(19)
H(24A)-C(24)-H(24C)	109.6(19)	C(26)-C(29)-H(29C)	110.3(13)
H(24B)-C(24)-H(24C)	103.8(19)	H(29A)-C(29)-H(29C)	109.6(17)
C(22)-C(25)-H(25A)	111.0(13)	H(29B)-C(29)-H(29C)	107.7(17)
C(22)-C(25)-H(25B)	109.7(12)	C(32)-C(30)-C(33)	107.72(19)

C(32)-C(30)-C(14)	111.92(16)	C(34)-C(35)-H(35A)	115.7(12)
C(33)-C(30)-C(14)	109.77(17)	C(34)-C(35)-H(35B)	110.4(12)
C(32)-C(30)-C(31)	109.04(19)	H(35A)-C(35)-H(35B)	106.5(17)
C(33)-C(30)-C(31)	108.91(19)	C(34)-C(35)-H(35C)	109.7(12)
C(14)-C(30)-C(31)	109.42(17)	H(35A)-C(35)-H(35C)	108.8(18)
C(30)-C(31)-H(31A)	107.7(14)	H(35B)-C(35)-H(35C)	105.3(17)
C(30)-C(31)-H(31B)	107.0(12)	C(34)-C(36)-H(36A)	109.0(13)
H(31A)-C(31)-H(31B)	113(2)	C(34)-C(36)-H(36B)	108.7(12)
C(30)-C(31)-H(31C)	110.9(12)	H(36A)-C(36)-H(36B)	107.4(18)
H(31A)-C(31)-H(31C)	106(2)	C(34)-C(36)-H(36C)	109.4(12)
H(31B)-C(31)-H(31C)	112.5(17)	H(36A)-C(36)-H(36C)	110.1(16)
C(30)-C(32)-H(32A)	109.2(14)	H(36B)-C(36)-H(36C)	112.2(16)
C(30)-C(32)-H(32B)	110.2(13)	C(34)-C(37)-H(37A)	113.9(12)
H(32A)-C(32)-H(32B)	105.9(18)	C(34)-C(37)-H(37B)	109.8(12)
C(30)-C(32)-H(32C)	111.3(14)	H(37A)-C(37)-H(37B)	102.9(17)
H(32A)-C(32)-H(32C)	110.7(18)	C(34)-C(37)-H(37C)	112.4(12)
H(32B)-C(32)-H(32C)	109.4(18)	H(37A)-C(37)-H(37C)	106.7(17)
C(30)-C(33)-H(33A)	109.9(16)	H(37B)-C(37)-H(37C)	110.7(19)
C(30)-C(33)-H(33B)	112.8(14)	C(39)-C(38)-C(43)	118.43(17)
H(33A)-C(33)-H(33B)	106.5(19)	C(39)-C(38)-P(1)	122.10(15)
C(30)-C(33)-H(33C)	112.4(15)	C(43)-C(38)-P(1)	119.44(15)
H(33A)-C(33)-H(33C)	106(2)	C(40)-C(39)-C(38)	120.4(2)
H(33B)-C(33)-H(33C)	109(2)	C(40)-C(39)-H(39)	118.2(11)
C(37)-C(34)-C(16)	111.66(16)	C(38)-C(39)-H(39)	121.4(11)
C(37)-C(34)-C(35)	107.39(17)	C(41)-C(40)-C(39)	120.6(2)
C(16)-C(34)-C(35)	109.54(17)	C(41)-C(40)-H(40)	121.6(12)
C(37)-C(34)-C(36)	107.05(18)	C(39)-C(40)-H(40)	117.7(12)
C(16)-C(34)-C(36)	110.78(16)	C(40)-C(41)-C(42)	119.70(19)
C(35)-C(34)-C(36)	110.34(17)	C(40)-C(41)-H(41)	120.6(16)

C(42)-C(41)-H(41)	119.7(16)	C(50)-C(51)-H(51)	120.0(14)
C(41)-C(42)-C(43)	120.1(2)	C(52)-C(51)-H(51)	118.3(14)
C(41)-C(42)-H(42)	121.8(13)	C(53)-C(52)-C(51)	119.7(2)
C(43)-C(42)-H(42)	118.2(13)	C(53)-C(52)-H(52)	123.5(16)
C(42)-C(43)-C(38)	120.7(2)	C(51)-C(52)-H(52)	116.1(16)
C(42)-C(43)-H(43)	120.0(11)	C(54)-C(53)-C(52)	120.3(2)
C(38)-C(43)-H(43)	119.3(11)	C(54)-C(53)-H(53)	122.7(15)
C(45)-C(44)-C(49)	118.12(19)	C(52)-C(53)-H(53)	117.0(15)
C(45)-C(44)-P(1)	125.81(15)	C(53)-C(54)-C(55)	120.3(2)
C(49)-C(44)-P(1)	116.06(14)	C(53)-C(54)-H(54)	119.2(15)
C(44)-C(45)-C(46)	120.81(19)	C(55)-C(54)-H(54)	120.5(15)
C(44)-C(45)-H(45)	119.6(13)	C(54)-C(55)-C(50)	120.5(2)
C(46)-C(45)-H(45)	119.6(13)	C(54)-C(55)-H(55)	119.6(14)
C(47)-C(46)-C(45)	120.4(2)	C(50)-C(55)-H(55)	119.9(14)
C(47)-C(46)-H(46)	118.7(12)	C(61)-C(56)-C(57)	118.80(17)
C(45)-C(46)-H(46)	120.9(12)	C(61)-C(56)-P(2)	120.48(14)
C(46)-C(47)-C(48)	119.8(2)	C(57)-C(56)-P(2)	120.55(15)
C(46)-C(47)-H(47)	117.7(13)	C(58)-C(57)-C(56)	120.6(2)
C(48)-C(47)-H(47)	122.5(13)	C(58)-C(57)-H(57)	122.4(12)
C(49)-C(48)-C(47)	120.0(2)	C(56)-C(57)-H(57)	117.0(12)
C(49)-C(48)-H(48)	119.8(12)	C(59)-C(58)-C(57)	120.0(2)
C(47)-C(48)-H(48)	120.1(12)	C(59)-C(58)-H(58)	122.2(15)
C(48)-C(49)-C(44)	120.84(19)	C(57)-C(58)-H(58)	117.8(15)
C(48)-C(49)-H(49)	120.0(13)	C(60)-C(59)-C(58)	120.07(19)
C(44)-C(49)-H(49)	119.1(13)	C(60)-C(59)-H(59)	117.8(13)
C(55)-C(50)-C(51)	118.9(2)	C(58)-C(59)-H(59)	122.0(13)
C(55)-C(50)-P(1)	120.68(15)	C(59)-C(60)-C(61)	119.8(2)
C(51)-C(50)-P(1)	120.09(17)	C(59)-C(60)-H(60)	122.2(11)
C(50)-C(51)-C(52)	120.2(2)	C(61)-C(60)-H(60)	118.0(11)

C(56)-C(61)-C(60)	120.75(19)	C(69)-C(70)-H(70)	120.9(13)
C(56)-C(61)-H(61)	119.5(12)	C(70)-C(71)-C(72)	119.9(2)
C(60)-C(61)-H(61)	119.8(12)	C(70)-C(71)-H(71)	119.2(13)
C(63)-C(62)-C(67)	118.14(19)	C(72)-C(71)-H(71)	120.9(13)
C(63)-C(62)-P(2)	115.40(14)	C(73)-C(72)-C(71)	119.8(2)
C(67)-C(62)-P(2)	126.40(16)	C(73)-C(72)-H(72)	119.0(12)
C(64)-C(63)-C(62)	121.01(19)	C(71)-C(72)-H(72)	121.2(12)
C(64)-C(63)-H(63)	121.1(13)	C(72)-C(73)-C(68)	121.24(18)
C(62)-C(63)-H(63)	117.9(13)	C(72)-C(73)-H(73)	114.4(13)
C(63)-C(64)-C(65)	119.9(2)	C(68)-C(73)-H(73)	124.3(13)
C(63)-C(64)-H(64)	119.2(15)	C(82)-C(81)-H(81A)	109.5
C(65)-C(64)-H(64)	120.7(15)	C(82)-C(81)-H(81B)	109.5
C(66)-C(65)-C(64)	119.7(2)	H(81A)-C(81)-H(81B)	109.5
C(66)-C(65)-H(65)	123.7(14)	C(82)-C(81)-H(81C)	109.5
C(64)-C(65)-H(65)	116.5(14)	H(81A)-C(81)-H(81C)	109.5
C(65)-C(66)-C(67)	120.7(2)	H(81B)-C(81)-H(81C)	109.5
C(65)-C(66)-H(66)	121.5(15)	C(83)-C(82)-C(81)	114.0(3)
C(67)-C(66)-H(66)	117.7(15)	C(83)-C(82)-H(82A)	108.8
C(66)-C(67)-C(62)	120.4(2)	C(81)-C(82)-H(82A)	108.8
C(66)-C(67)-H(67)	119.6(13)	C(83)-C(82)-H(82B)	108.8
C(62)-C(67)-H(67)	119.9(13)	C(81)-C(82)-H(82B)	108.8
C(69)-C(68)-C(73)	118.09(18)	H(82A)-C(82)-H(82B)	107.7
C(69)-C(68)-P(2)	123.37(15)	C(84)-C(83)-C(82)	117.4(3)
C(73)-C(68)-P(2)	118.45(13)	C(84)-C(83)-H(83A)	108.0
C(70)-C(69)-C(68)	120.30(19)	C(82)-C(83)-H(83A)	108.0
C(70)-C(69)-H(69)	121.0(11)	C(84)-C(83)-H(83B)	108.0
C(68)-C(69)-H(69)	118.7(11)	C(82)-C(83)-H(83B)	108.0
C(71)-C(70)-C(69)	120.66(19)	H(83A)-C(83)-H(83B)	107.2
C(71)-C(70)-H(70)	118.5(13)	C(85)-C(84)-C(83)	116.2(4)

C(85)-C(84)-H(84A)	108.2
C(83)-C(84)-H(84A)	108.2
C(85)-C(84)-H(84B)	108.2
C(83)-C(84)-H(84B)	108.2
H(84A)-C(84)-H(84B)	107.4
C(84)-C(85)-H(85A)	109.5
C(84)-C(85)-H(85B)	109.5
H(85A)-C(85)-H(85B)	109.5
C(84)-C(85)-H(85C)	109.5
H(85A)-C(85)-H(85C)	109.5
H(85B)-C(85)-H(85C)	109.5

Table S36. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	127(1)	115(1)	111(1)	0(1)	24(1)	18(1)
P(1)	170(2)	140(2)	156(3)	26(2)	62(2)	35(2)
P(2)	144(2)	117(2)	123(2)	-7(2)	21(2)	4(2)
O(1)	123(5)	146(7)	191(8)	-24(5)	39(5)	5(5)
O(2)	134(5)	153(7)	159(7)	29(5)	49(5)	42(5)
N(1)	123(6)	106(8)	129(8)	4(6)	35(6)	-6(5)
C(1)	146(8)	127(9)	147(10)	16(7)	36(7)	-3(7)
C(2)	138(8)	160(9)	148(10)	29(8)	21(7)	4(7)
C(3)	125(8)	183(10)	189(11)	43(8)	60(7)	27(7)
C(4)	166(8)	140(10)	170(10)	31(7)	78(7)	17(7)
C(5)	156(8)	134(9)	132(10)	2(7)	43(7)	-19(7)
C(6)	120(8)	133(9)	142(10)	11(7)	46(7)	5(6)
C(7)	121(8)	105(9)	148(10)	4(7)	38(7)	-20(6)
C(8)	125(8)	143(9)	157(11)	-19(7)	65(7)	-11(7)
C(9)	137(8)	120(9)	139(10)	11(7)	29(7)	-25(6)
C(10)	93(7)	146(9)	158(10)	4(8)	22(6)	-4(7)
C(11)	115(7)	111(9)	143(10)	10(7)	35(6)	-3(6)
C(12)	108(7)	131(9)	142(10)	-21(7)	25(7)	0(6)
C(13)	168(8)	137(9)	121(10)	-2(7)	25(7)	1(7)
C(14)	143(8)	136(9)	167(11)	-19(7)	18(7)	13(7)
C(15)	137(8)	173(10)	203(11)	-42(8)	70(7)	15(7)
C(16)	172(8)	139(9)	160(11)	-20(7)	68(7)	-4(7)
C(17)	140(8)	102(9)	156(10)	-27(7)	43(7)	7(6)
C(18)	124(7)	204(10)	234(11)	-25(9)	19(7)	1(8)

C(19)	197(10)	209(11)	256(13)	-28(9)	52(9)	-54(8)
C(20)	185(9)	252(12)	220(12)	-5(9)	-27(8)	29(9)
C(21)	142(9)	350(15)	377(16)	-96(11)	38(9)	-20(9)
C(22)	189(9)	150(10)	208(11)	13(8)	98(8)	27(7)
C(23)	485(15)	198(12)	300(15)	28(10)	145(12)	119(11)
C(24)	285(11)	235(12)	344(15)	-14(11)	202(10)	17(9)
C(25)	275(11)	251(12)	354(15)	-120(11)	137(10)	-12(9)
C(26)	144(8)	194(10)	130(10)	-13(8)	20(7)	-4(7)
C(27)	286(11)	277(12)	183(13)	39(9)	36(9)	23(9)
C(28)	184(10)	281(12)	204(13)	-77(10)	28(9)	-46(9)
C(29)	210(10)	350(14)	153(12)	-43(10)	41(9)	24(9)
C(30)	171(8)	188(10)	240(12)	7(9)	35(8)	55(7)
C(31)	172(10)	312(14)	391(16)	103(12)	44(10)	58(9)
C(32)	198(10)	232(12)	313(14)	67(10)	11(9)	56(9)
C(33)	411(14)	279(13)	350(16)	-17(11)	58(12)	191(11)
C(34)	184(8)	195(11)	205(11)	26(8)	96(8)	40(7)
C(35)	245(11)	197(11)	279(14)	30(9)	98(10)	-8(8)
C(36)	295(11)	226(12)	162(11)	13(9)	84(8)	52(8)
C(37)	239(10)	354(14)	324(14)	90(12)	173(10)	52(10)
C(38)	186(8)	140(9)	170(10)	38(8)	33(7)	29(7)
C(39)	209(9)	167(10)	184(12)	34(8)	47(8)	21(7)
C(40)	214(10)	236(11)	276(13)	43(9)	92(9)	65(8)
C(41)	202(10)	293(12)	316(14)	103(10)	35(9)	80(9)
C(42)	263(10)	334(14)	212(13)	90(10)	6(9)	38(9)
C(43)	259(10)	250(12)	193(11)	31(9)	76(8)	37(9)
C(44)	193(9)	131(9)	186(11)	26(8)	85(8)	-11(7)
C(45)	193(9)	154(10)	255(12)	34(8)	68(8)	8(7)
C(46)	325(11)	135(10)	294(14)	-18(9)	115(10)	1(8)
C(47)	366(12)	195(11)	274(14)	-13(10)	12(10)	-79(9)

C(48)	245(10)	211(11)	327(14)	29(10)	-31(9)	-34(8)
C(49)	182(9)	140(10)	292(12)	19(9)	54(8)	-3(7)
C(50)	184(8)	205(11)	210(11)	69(8)	63(8)	63(7)
C(51)	269(10)	236(12)	310(14)	41(10)	140(10)	35(9)
C(52)	337(12)	284(13)	427(17)	121(11)	195(11)	42(10)
C(53)	247(11)	400(14)	318(15)	115(11)	180(10)	112(10)
C(54)	235(10)	393(14)	200(13)	42(11)	76(9)	111(9)
C(55)	192(9)	290(12)	189(12)	42(9)	38(8)	61(8)
C(56)	137(8)	166(10)	143(10)	-42(7)	35(7)	-10(7)
C(57)	220(9)	174(11)	193(12)	-13(8)	4(8)	0(8)
C(58)	207(10)	271(12)	247(13)	-29(9)	-56(9)	16(8)
C(59)	192(9)	249(12)	322(14)	-86(10)	0(9)	-56(8)
C(60)	240(10)	178(11)	347(14)	-13(10)	32(9)	-48(8)
C(61)	177(9)	180(10)	244(12)	2(8)	10(8)	-1(7)
C(62)	146(8)	142(9)	156(10)	17(8)	0(7)	-36(7)
C(63)	202(9)	152(10)	182(11)	-1(8)	39(8)	-34(7)
C(64)	282(11)	268(12)	174(12)	-12(9)	65(9)	-93(9)
C(65)	275(10)	304(13)	179(12)	92(10)	-32(9)	-91(9)
C(66)	186(9)	218(11)	303(14)	110(10)	-20(9)	-2(8)
C(67)	189(9)	175(10)	214(12)	17(9)	33(8)	-12(7)
C(68)	178(8)	98(9)	155(10)	1(7)	49(7)	-5(7)
C(69)	215(9)	132(10)	191(12)	-18(8)	32(8)	-4(7)
C(70)	220(9)	154(10)	292(13)	-11(9)	106(9)	13(8)
C(71)	305(11)	166(10)	284(13)	-45(9)	181(10)	-20(8)
C(72)	293(10)	221(11)	172(12)	-33(9)	70(9)	-57(8)
C(73)	200(9)	189(10)	184(11)	-13(8)	45(8)	-28(8)
C(81)	480(16)	690(20)	680(20)	-34(18)	172(16)	-19(15)
C(82)	710(20)	650(20)	600(20)	96(18)	263(17)	10(17)

C(83)	651(18)	453(18)	480(20)	-117(14)	270(15)	-13(13)
C(84)	720(20)	970(30)	720(30)	-360(20)	391(19)	-230(20)
C(85)	1000(30)	900(30)	1480(50)	-640(30)	690(30)	-430(20)

Table S37. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **11**.

	x	y	z	U_{iso}
H(1)	6678(11)	9321(8)	6233(13)	30
H(3)	4109(11)	10243(8)	8405(12)	17(5)
H(5)	6472(10)	10571(8)	9363(12)	12(5)
H(8)	7167(10)	9889(7)	10005(11)	7(5)
H(10)	9253(11)	9264(8)	9669(12)	16(5)
H(13)	9437(9)	8543(7)	9010(11)	2(4)
H(15)	10623(10)	8766(8)	7250(12)	12(5)
H(19A)	4930(11)	8615(8)	7664(12)	17(5)
H(19B)	4008(12)	8522(9)	7422(14)	28(6)
H(19C)	4340(12)	8695(9)	8289(15)	30(6)
H(20A)	4085(11)	9817(9)	6437(13)	24(6)
H(20B)	3893(12)	9187(9)	6283(14)	29(6)
H(20C)	4787(12)	9405(8)	6497(13)	23(6)
H(21A)	3319(12)	9449(9)	8101(15)	27(6)
H(21B)	3020(12)	9264(9)	7242(14)	28(6)
H(21C)	3228(11)	9905(9)	7416(13)	24(6)
H(23A)	4990(12)	11588(9)	8456(14)	33(7)
H(23B)	4419(13)	11768(11)	9017(15)	44(7)
H(23C)	4123(13)	11317(10)	8403(15)	37(7)
H(24A)	3851(13)	10710(9)	9477(14)	31(6)
H(24B)	4193(11)	11172(9)	10159(14)	29(6)
H(24C)	4526(12)	10568(10)	10192(15)	33(7)
H(25A)	5929(12)	11022(10)	10365(14)	31(6)
H(25B)	5483(12)	11591(9)	10212(14)	31(6)
H(25C)	6104(12)	11427(9)	9685(14)	34(6)

H(27A)	8471(13)	8830(10)	11158(14)	35(7)
H(27B)	9187(13)	9073(10)	11756(16)	37(7)
H(27C)	9326(12)	8858(9)	10933(13)	27(6)
H(28A)	9832(12)	9859(9)	10702(13)	23(6)
H(28B)	9681(11)	10049(8)	11496(14)	20(6)
H(28C)	9291(11)	10373(9)	10782(13)	23(6)
H(29A)	7970(12)	10233(10)	11192(14)	28(6)
H(29B)	8394(11)	9906(8)	11915(14)	20(6)
H(29C)	7639(12)	9660(9)	11329(13)	23(6)
H(31A)	11560(12)	8644(10)	9182(15)	32(7)
H(31B)	11724(11)	8576(9)	8347(14)	22(6)
H(31C)	12025(12)	8129(9)	9038(13)	32(6)
H(32A)	10545(11)	8058(9)	9623(14)	27(6)
H(32B)	10987(11)	7540(9)	9443(13)	24(6)
H(32C)	10074(12)	7613(9)	9084(13)	28(6)
H(33A)	11276(14)	7394(11)	8120(16)	53(8)
H(33B)	10988(13)	7833(10)	7427(16)	40(7)
H(33C)	10343(15)	7448(11)	7743(16)	51(8)
H(35A)	9023(12)	10241(9)	6561(13)	25(6)
H(35B)	9601(11)	10345(9)	5965(14)	25(6)
H(35C)	9951(11)	10267(8)	6857(13)	15(5)
H(36A)	9166(11)	8906(10)	5532(13)	28(6)
H(36B)	9081(11)	9512(9)	5165(14)	25(6)
H(36C)	8486(11)	9298(8)	5741(12)	17(5)
H(37A)	10935(11)	9555(8)	6577(13)	18(6)
H(37B)	10554(12)	9637(10)	5718(15)	32(6)
H(37C)	10619(11)	9036(9)	6106(13)	21(6)
H(39)	5504(10)	10771(7)	7497(12)	5(5)
H(40)	4235(11)	11094(8)	7027(13)	21(6)

H(41)	3735(13)	11077(9)	5672(15)	38(7)
H(42)	4524(11)	10711(9)	4854(14)	24(6)
H(43)	5844(10)	10430(7)	5353(11)	8(5)
H(45)	6492(11)	11417(8)	7577(12)	18(5)
H(46)	7126(10)	11947(9)	8648(12)	21(6)
H(47)	8366(12)	11692(9)	9354(14)	31(6)
H(48)	9060(11)	10898(8)	8989(13)	22(6)
H(49)	8378(11)	10356(9)	7942(13)	23(6)
H(51)	7792(12)	11286(9)	6489(14)	32(7)
H(52)	8234(13)	11588(11)	5415(15)	48(8)
H(53)	8098(12)	10993(9)	4319(14)	33(7)
H(54)	7592(13)	10088(10)	4371(15)	36(7)
H(55)	7112(12)	9763(10)	5467(14)	34(6)
H(57)	5620(10)	8671(9)	6188(12)	17(5)
H(58)	4465(12)	8174(10)	5633(14)	35(7)
H(59)	4247(12)	7243(9)	6025(13)	33(6)
H(60)	5303(10)	6824(9)	6951(12)	19(5)
H(61)	6473(11)	7328(8)	7471(12)	20(5)
H(63)	6777(10)	8553(8)	8662(12)	14(5)
H(64)	7067(11)	8157(9)	9871(14)	27(6)
H(65)	7963(11)	7456(9)	10134(14)	23(6)
H(66)	8577(11)	7117(9)	9153(13)	23(6)
H(67)	8225(10)	7472(8)	7948(12)	14(5)
H(69)	8819(10)	8080(8)	7241(12)	10(5)
H(70)	9557(11)	7745(8)	6331(12)	22(6)
H(71)	8854(11)	7616(8)	5071(13)	19(5)
H(72)	7473(10)	7830(8)	4685(13)	17(5)
H(73)	6767(11)	8142(9)	5542(13)	26(6)

H(81A)	5244	7300	9466	91
H(81B)	5369	7750	8823	91
H(81C)	5561	7102	8708	91
H(82A)	3977	7539	8676	76
H(82B)	4292	7366	7909	76
H(83A)	4386	6430	8323	61
H(83B)	4080	6601	9093	61
H(84A)	2813	6855	8280	92
H(84B)	3131	6607	7552	92
H(85A)	3211	5726	8129	160
H(85B)	2306	5973	7950	160
H(85C)	2843	5983	8824	160

$(ONO^{tBu})Ir(PPh_3)_2Me$, 12

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S38. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **12**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	8756(1)	1679(1)	7695(1)	11(1)
P(1)	7756(1)	818(1)	7269(1)	13(1)
P(2)	9650(1)	2637(1)	8035(1)	13(1)
O(1)	7754(1)	1642(1)	8305(1)	13(1)
O(2)	9798(2)	1670(1)	7119(1)	15(1)
N(1)	9817(2)	1140(1)	8294(1)	12(1)
C(1)	8115(2)	1698(1)	8881(1)	11(1)
C(2)	7418(2)	1837(1)	9279(1)	12(1)
C(3)	7832(2)	2069(1)	9839(1)	13(1)
C(4)	8894(2)	2141(1)	10057(1)	13(1)
C(5)	9527(2)	1886(1)	9706(1)	14(1)
C(6)	9173(2)	1630(1)	9140(1)	10(1)
C(7)	9884(2)	1217(1)	8888(1)	12(1)
C(8)	10600(2)	870(1)	9284(1)	14(1)
C(9)	11315(2)	473(1)	9094(2)	14(1)
C(10)	11249(2)	424(1)	8490(2)	14(1)
C(11)	10485(2)	735(1)	8094(1)	13(1)
C(12)	10450(2)	636(1)	7452(1)	13(1)
C(13)	10759(2)	29(1)	7281(2)	16(1)
C(14)	10991(2)	-92(1)	6735(2)	16(1)
C(15)	10959(2)	432(1)	6348(2)	17(1)
C(16)	10602(2)	1032(1)	6468(1)	14(1)
C(17)	10260(2)	1125(1)	7020(1)	14(1)
C(18)	6252(2)	1732(1)	9099(1)	16(1)

C(19)	6045(2)	1057(1)	8840(2)	20(1)
C(20)	5773(2)	2242(1)	8648(2)	20(1)
C(21)	5706(2)	1768(1)	9637(2)	23(1)
C(22)	9282(2)	2453(1)	10660(2)	16(1)
C(23)	8880(3)	3140(1)	10650(2)	23(1)
C(24)	8911(3)	2072(1)	11153(2)	21(1)
C(25)	10461(2)	2483(1)	10794(2)	21(1)
C(26)	12109(2)	117(1)	9551(2)	17(1)
C(27)	12835(3)	-277(2)	9257(2)	32(1)
C(28)	12736(3)	596(1)	9976(2)	30(1)
C(29)	11520(3)	-326(1)	9902(2)	24(1)
C(30)	11314(2)	-755(1)	6542(2)	18(1)
C(31)	10664(3)	-934(1)	5943(2)	25(1)
C(32)	12453(2)	-732(1)	6493(2)	23(1)
C(33)	11170(3)	-1275(1)	6992(2)	25(1)
C(34)	10620(2)	1586(1)	6026(1)	18(1)
C(35)	9559(3)	1901(1)	5840(2)	27(1)
C(36)	10969(3)	1362(1)	5460(2)	24(1)
C(37)	11396(3)	2080(1)	6331(2)	26(1)
C(38)	6385(2)	830(1)	7326(2)	16(1)
C(39)	5827(2)	1393(1)	7340(1)	18(1)
C(40)	4771(3)	1378(1)	7323(2)	22(1)
C(41)	4249(3)	806(2)	7301(2)	26(1)
C(42)	4800(3)	248(2)	7300(2)	29(1)
C(43)	5839(2)	263(1)	7306(2)	22(1)
C(44)	8133(2)	39(1)	7596(1)	13(1)
C(45)	8200(2)	-511(1)	7267(2)	18(1)
C(46)	8500(2)	-1083(1)	7553(2)	21(1)
C(47)	8719(3)	-1113(1)	8159(2)	23(1)

C(48)	8635(3)	-573(1)	8493(2)	23(1)
C(49)	8338(2)	1(1)	8212(2)	18(1)
C(50)	7641(2)	706(1)	6462(1)	14(1)
C(51)	6780(3)	940(1)	6073(2)	19(1)
C(52)	6703(3)	889(1)	5464(2)	22(1)
C(53)	7486(3)	605(1)	5229(2)	23(1)
C(54)	8336(3)	365(1)	5608(2)	21(1)
C(55)	8412(3)	421(1)	6215(2)	18(1)
C(56)	9099(2)	3237(1)	8470(1)	15(1)
C(57)	8165(2)	3147(1)	8654(1)	16(1)
C(58)	7821(3)	3590(1)	9027(2)	23(1)
C(59)	8401(3)	4124(1)	9202(2)	24(1)
C(60)	9302(3)	4237(1)	8998(2)	23(1)
C(61)	9652(3)	3799(1)	8632(2)	20(1)
C(62)	10918(2)	2488(1)	8492(2)	15(1)
C(63)	11633(2)	2119(1)	8256(2)	21(1)
C(64)	12600(3)	2002(1)	8587(2)	27(1)
C(65)	12865(3)	2241(2)	9153(2)	30(1)
C(66)	12167(3)	2594(1)	9406(2)	26(1)
C(67)	11199(3)	2713(1)	9073(2)	19(1)
C(68)	9932(2)	3171(1)	7445(2)	15(1)
C(69)	9119(2)	3531(1)	7136(2)	18(1)
C(70)	9267(3)	3939(1)	6685(2)	23(1)
C(71)	10225(3)	4007(1)	6539(2)	26(1)
C(72)	11044(3)	3671(1)	6849(2)	24(1)
C(73)	10898(2)	3254(1)	7302(2)	19(1)
C(74)	7792(2)	2240(1)	7070(1)	17(1)

Table S39. Selected bond lengths [Å] and angles [°] for 12.

Ir(1)-O(2)	2.0700(19)	O(2)-Ir(1)-O(1)	176.50(8)
Ir(1)-O(1)	2.0901(19)	O(2)-Ir(1)-C(74)	87.80(10)
Ir(1)-C(74)	2.095(3)	O(1)-Ir(1)-C(74)	95.59(10)
Ir(1)-N(1)	2.104(2)	O(2)-Ir(1)-N(1)	88.21(9)
Ir(1)-P(1)	2.3449(8)	O(1)-Ir(1)-N(1)	88.43(9)
Ir(1)-P(2)	2.3895(8)	C(74)-Ir(1)-N(1)	175.67(11)
		O(2)-Ir(1)-P(1)	96.70(6)
		O(1)-Ir(1)-P(1)	82.69(6)
		C(74)-Ir(1)-P(1)	85.58(8)
		N(1)-Ir(1)-P(1)	96.55(7)
		O(2)-Ir(1)-P(2)	82.47(6)
		O(1)-Ir(1)-P(2)	98.56(6)
		C(74)-Ir(1)-P(2)	87.31(8)
		N(1)-Ir(1)-P(2)	90.50(7)
		P(1)-Ir(1)-P(2)	172.87(3)

Table S40. Bond lengths [Å] and angles [°] for **12**.

Ir(1)-O(2)	2.0700(19)	P(1)-C(50)	1.840(3)
Ir(1)-O(1)	2.0901(19)	P(2)-C(62)	1.833(3)
Ir(1)-C(74)	2.095(3)	P(2)-C(56)	1.836(3)
Ir(1)-N(1)	2.104(2)	P(2)-C(68)	1.845(3)
Ir(1)-P(1)	2.3449(8)	O(1)-C(1)	1.322(3)
Ir(1)-P(2)	2.3895(8)	O(2)-C(17)	1.335(3)
P(1)-C(44)	1.830(3)	N(1)-C(7)	1.356(4)
P(1)-C(38)	1.838(3)	N(1)-C(11)	1.361(4)

C(1)-C(6)	1.422(4)	C(26)-C(27)	1.514(4)
C(1)-C(2)	1.437(4)	C(26)-C(29)	1.530(4)
C(2)-C(3)	1.387(4)	C(26)-C(28)	1.533(4)
C(2)-C(18)	1.536(4)	C(30)-C(32)	1.529(4)
C(3)-C(4)	1.409(4)	C(30)-C(31)	1.527(4)
C(4)-C(5)	1.368(4)	C(30)-C(33)	1.535(4)
C(4)-C(22)	1.529(4)	C(34)-C(36)	1.524(4)
C(5)-C(6)	1.403(4)	C(34)-C(37)	1.534(4)
C(6)-C(7)	1.470(4)	C(34)-C(35)	1.537(4)
C(7)-C(8)	1.392(4)	C(38)-C(43)	1.389(4)
C(8)-C(9)	1.386(4)	C(38)-C(39)	1.395(4)
C(9)-C(10)	1.374(4)	C(39)-C(40)	1.388(4)
C(9)-C(26)	1.534(4)	C(40)-C(41)	1.381(4)
C(10)-C(11)	1.393(4)	C(41)-C(42)	1.381(4)
C(11)-C(12)	1.476(4)	C(42)-C(43)	1.370(4)
C(12)-C(17)	1.415(4)	C(44)-C(45)	1.390(4)
C(12)-C(13)	1.413(4)	C(44)-C(49)	1.388(4)
C(13)-C(14)	1.364(4)	C(45)-C(46)	1.391(4)
C(14)-C(15)	1.407(4)	C(46)-C(47)	1.365(5)
C(14)-C(30)	1.544(4)	C(47)-C(48)	1.383(4)
C(15)-C(16)	1.389(4)	C(48)-C(49)	1.389(4)
C(16)-C(17)	1.431(4)	C(50)-C(55)	1.386(4)
C(16)-C(34)	1.545(4)	C(50)-C(51)	1.400(4)
C(18)-C(19)	1.542(4)	C(51)-C(52)	1.384(4)
C(18)-C(21)	1.536(4)	C(52)-C(53)	1.383(5)
C(18)-C(20)	1.541(4)	C(53)-C(54)	1.382(5)
C(22)-C(25)	1.532(4)	C(54)-C(55)	1.380(4)
C(22)-C(24)	1.533(4)	C(56)-C(57)	1.386(4)
C(22)-C(23)	1.537(4)	C(56)-C(61)	1.402(4)

C(57)-C(58)	1.392(4)	C(74)-Ir(1)-P(2)	87.31(8)
C(58)-C(59)	1.377(4)	N(1)-Ir(1)-P(2)	90.50(7)
C(59)-C(60)	1.373(5)	P(1)-Ir(1)-P(2)	172.87(3)
C(60)-C(61)	1.379(4)	C(44)-P(1)-C(38)	100.51(13)
C(62)-C(67)	1.396(4)	C(44)-P(1)-C(50)	105.32(14)
C(62)-C(63)	1.401(4)	C(38)-P(1)-C(50)	99.69(15)
C(63)-C(64)	1.384(4)	C(44)-P(1)-Ir(1)	115.37(10)
C(64)-C(65)	1.374(5)	C(38)-P(1)-Ir(1)	116.54(10)
C(65)-C(66)	1.387(5)	C(50)-P(1)-Ir(1)	116.98(9)
C(66)-C(67)	1.386(4)	C(62)-P(2)-C(56)	102.56(14)
C(68)-C(73)	1.383(4)	C(62)-P(2)-C(68)	103.72(14)
C(68)-C(69)	1.395(4)	C(56)-P(2)-C(68)	97.56(13)
C(69)-C(70)	1.383(4)	C(62)-P(2)-Ir(1)	112.92(9)
C(70)-C(71)	1.372(5)	C(56)-P(2)-Ir(1)	122.25(10)
C(71)-C(72)	1.376(5)	C(68)-P(2)-Ir(1)	115.22(10)
C(72)-C(73)	1.397(4)	C(1)-O(1)-Ir(1)	120.24(17)
		C(17)-O(2)-Ir(1)	119.42(18)
O(2)-Ir(1)-O(1)	176.50(8)	C(7)-N(1)-C(11)	118.9(3)
O(2)-Ir(1)-C(74)	87.80(10)	C(7)-N(1)-Ir(1)	120.24(19)
O(1)-Ir(1)-C(74)	95.59(10)	C(11)-N(1)-Ir(1)	120.8(2)
O(2)-Ir(1)-N(1)	88.21(9)	O(1)-C(1)-C(6)	123.8(3)
O(1)-Ir(1)-N(1)	88.43(9)	O(1)-C(1)-C(2)	119.5(3)
C(74)-Ir(1)-N(1)	175.67(11)	C(6)-C(1)-C(2)	116.7(3)
O(2)-Ir(1)-P(1)	96.70(6)	C(3)-C(2)-C(1)	117.8(3)
O(1)-Ir(1)-P(1)	82.69(6)	C(3)-C(2)-C(18)	120.5(3)
C(74)-Ir(1)-P(1)	85.58(8)	C(1)-C(2)-C(18)	121.7(3)
N(1)-Ir(1)-P(1)	96.55(7)	C(2)-C(3)-C(4)	124.5(3)
O(2)-Ir(1)-P(2)	82.47(6)	C(5)-C(4)-C(3)	115.1(3)
O(1)-Ir(1)-P(2)	98.56(6)	C(5)-C(4)-C(22)	123.8(3)

C(3)-C(4)-C(22)	121.0(3)	C(12)-C(17)-C(16)	118.2(3)
C(4)-C(5)-C(6)	123.7(3)	C(2)-C(18)-C(19)	109.6(2)
C(5)-C(6)-C(1)	119.1(3)	C(2)-C(18)-C(21)	111.7(3)
C(5)-C(6)-C(7)	117.2(3)	C(19)-C(18)-C(21)	106.2(2)
C(1)-C(6)-C(7)	122.9(3)	C(2)-C(18)-C(20)	110.4(2)
N(1)-C(7)-C(8)	120.3(3)	C(19)-C(18)-C(20)	111.0(3)
N(1)-C(7)-C(6)	122.2(3)	C(21)-C(18)-C(20)	107.9(2)
C(8)-C(7)-C(6)	117.4(3)	C(25)-C(22)-C(24)	108.8(3)
C(9)-C(8)-C(7)	122.1(3)	C(25)-C(22)-C(4)	111.2(3)
C(10)-C(9)-C(8)	116.0(3)	C(24)-C(22)-C(4)	110.0(2)
C(10)-C(9)-C(26)	124.1(3)	C(25)-C(22)-C(23)	107.4(2)
C(8)-C(9)-C(26)	119.9(3)	C(24)-C(22)-C(23)	110.1(3)
C(9)-C(10)-C(11)	121.8(3)	C(4)-C(22)-C(23)	109.3(3)
N(1)-C(11)-C(10)	120.7(3)	C(27)-C(26)-C(29)	108.8(3)
N(1)-C(11)-C(12)	121.2(3)	C(27)-C(26)-C(28)	109.1(3)
C(10)-C(11)-C(12)	118.1(3)	C(29)-C(26)-C(28)	109.5(3)
C(17)-C(12)-C(13)	119.0(3)	C(27)-C(26)-C(9)	111.9(3)
C(17)-C(12)-C(11)	124.1(3)	C(29)-C(26)-C(9)	107.8(3)
C(13)-C(12)-C(11)	116.3(3)	C(28)-C(26)-C(9)	109.7(2)
C(14)-C(13)-C(12)	123.0(3)	C(32)-C(30)-C(31)	110.0(3)
C(13)-C(14)-C(15)	116.3(3)	C(32)-C(30)-C(33)	108.4(3)
C(13)-C(14)-C(30)	123.3(3)	C(31)-C(30)-C(33)	108.0(3)
C(15)-C(14)-C(30)	120.3(3)	C(32)-C(30)-C(14)	108.5(2)
C(16)-C(15)-C(14)	123.9(3)	C(31)-C(30)-C(14)	109.8(3)
C(15)-C(16)-C(17)	118.0(3)	C(33)-C(30)-C(14)	112.1(3)
C(15)-C(16)-C(34)	120.6(3)	C(36)-C(34)-C(37)	108.4(3)
C(17)-C(16)-C(34)	121.3(3)	C(36)-C(34)-C(35)	107.3(3)
O(2)-C(17)-C(12)	122.2(3)	C(37)-C(34)-C(35)	109.5(3)
O(2)-C(17)-C(16)	119.5(3)	C(36)-C(34)-C(16)	111.5(2)

C(37)-C(34)-C(16)	107.4(3)	C(56)-C(57)-C(58)	120.1(3)
C(35)-C(34)-C(16)	112.7(3)	C(59)-C(58)-C(57)	119.8(3)
C(43)-C(38)-C(39)	117.1(3)	C(60)-C(59)-C(58)	120.8(3)
C(43)-C(38)-P(1)	119.8(2)	C(59)-C(60)-C(61)	119.8(3)
C(39)-C(38)-P(1)	123.0(2)	C(60)-C(61)-C(56)	120.4(3)
C(40)-C(39)-C(38)	120.8(3)	C(67)-C(62)-C(63)	118.2(3)
C(41)-C(40)-C(39)	120.8(3)	C(67)-C(62)-P(2)	122.9(2)
C(40)-C(41)-C(42)	118.6(3)	C(63)-C(62)-P(2)	118.9(3)
C(43)-C(42)-C(41)	120.5(3)	C(64)-C(63)-C(62)	120.4(3)
C(42)-C(43)-C(38)	122.2(3)	C(65)-C(64)-C(63)	120.2(3)
C(45)-C(44)-C(49)	118.9(3)	C(64)-C(65)-C(66)	120.8(3)
C(45)-C(44)-P(1)	124.0(3)	C(67)-C(66)-C(65)	118.9(4)
C(49)-C(44)-P(1)	117.1(2)	C(66)-C(67)-C(62)	121.5(3)
C(44)-C(45)-C(46)	120.2(3)	C(73)-C(68)-C(69)	118.0(3)
C(47)-C(46)-C(45)	120.6(3)	C(73)-C(68)-P(2)	124.4(2)
C(46)-C(47)-C(48)	119.9(3)	C(69)-C(68)-P(2)	117.5(2)
C(47)-C(48)-C(49)	120.0(3)	C(70)-C(69)-C(68)	120.9(3)
C(44)-C(49)-C(48)	120.4(3)	C(71)-C(70)-C(69)	120.4(3)
C(55)-C(50)-C(51)	117.6(3)	C(70)-C(71)-C(72)	119.7(3)
C(55)-C(50)-P(1)	122.0(3)	C(71)-C(72)-C(73)	120.2(3)
C(51)-C(50)-P(1)	120.3(2)	C(68)-C(73)-C(72)	120.7(3)
C(52)-C(51)-C(50)	121.2(3)		
C(53)-C(52)-C(51)	120.0(3)		
C(52)-C(53)-C(54)	119.5(3)		
C(55)-C(54)-C(53)	120.3(3)		
C(50)-C(55)-C(54)	121.4(3)		
C(57)-C(56)-C(61)	118.9(3)		
C(57)-C(56)-P(2)	122.2(2)		
C(61)-C(56)-P(2)	118.9(2)		

Table S41. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **12**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	111(1)	107(1)	117(1)	2(1)	19(1)	0(1)
P(1)	138(5)	129(4)	117(5)	-10(3)	10(4)	-10(3)
P(2)	111(4)	122(4)	158(5)	8(4)	22(4)	-5(3)
O(1)	117(11)	158(11)	106(12)	-10(11)	2(10)	9(10)
O(2)	166(11)	152(10)	150(12)	27(11)	49(10)	15(10)
N(1)	129(14)	102(13)	139(16)	13(11)	15(13)	-2(10)
C(1)	119(14)	64(14)	135(17)	-16(15)	4(14)	-24(13)
C(2)	117(16)	79(16)	149(19)	0(12)	5(15)	5(11)
C(3)	114(16)	137(16)	160(20)	-8(14)	54(16)	29(12)
C(4)	152(17)	109(16)	116(19)	15(13)	-18(16)	16(12)
C(5)	106(16)	121(16)	170(20)	32(13)	-4(16)	21(11)
C(6)	80(14)	114(15)	98(17)	10(14)	-2(13)	6(13)
C(7)	108(16)	122(16)	137(19)	-6(14)	40(16)	-31(12)
C(8)	191(18)	137(17)	78(19)	-23(14)	12(16)	-10(13)
C(9)	157(17)	102(16)	150(20)	13(13)	22(16)	-1(12)
C(10)	154(17)	126(16)	160(20)	0(14)	27(16)	11(12)
C(11)	97(16)	143(17)	140(20)	10(14)	0(16)	-17(12)
C(12)	114(16)	136(16)	140(20)	-24(14)	29(16)	-6(12)
C(13)	144(17)	174(17)	160(20)	5(15)	10(16)	4(13)
C(14)	125(17)	155(17)	190(20)	-23(15)	-2(16)	-2(13)
C(15)	138(18)	267(19)	100(20)	-47(15)	13(16)	-18(13)
C(16)	130(17)	193(17)	100(19)	-19(14)	10(16)	-21(13)
C(17)	111(16)	132(17)	150(20)	-32(14)	-16(16)	-27(12)
C(18)	100(15)	190(17)	187(19)	5(16)	34(15)	9(14)

C(19)	123(18)	260(19)	190(20)	5(15)	-19(17)	-18(14)
C(20)	150(18)	179(18)	260(20)	-18(15)	-32(18)	13(13)
C(21)	120(16)	310(20)	250(20)	-38(17)	46(16)	2(14)
C(22)	186(18)	147(17)	130(20)	-33(14)	-4(16)	15(13)
C(23)	270(20)	220(19)	180(20)	-72(14)	25(18)	17(14)
C(24)	215(19)	247(19)	150(20)	-12(15)	6(17)	7(14)
C(25)	230(20)	197(18)	180(20)	-38(15)	-6(18)	-22(14)
C(26)	168(18)	195(18)	130(20)	6(14)	-10(16)	65(13)
C(27)	320(20)	410(20)	240(20)	73(18)	40(20)	246(17)
C(28)	200(20)	350(20)	310(30)	68(18)	-56(19)	55(16)
C(29)	240(20)	241(19)	210(20)	70(15)	-7(18)	95(14)
C(30)	174(18)	199(18)	160(20)	-46(15)	21(17)	24(13)
C(31)	260(20)	254(19)	250(20)	-49(16)	39(19)	42(15)
C(32)	208(19)	262(19)	220(20)	-77(16)	36(18)	56(15)
C(33)	310(20)	213(19)	230(20)	-86(16)	45(19)	44(15)
C(34)	198(17)	214(19)	149(19)	16(15)	46(16)	-31(14)
C(35)	300(20)	300(20)	220(20)	115(16)	70(20)	9(15)
C(36)	310(20)	236(19)	190(20)	14(15)	67(19)	-44(15)
C(37)	330(20)	260(20)	220(20)	-13(16)	110(20)	-92(16)
C(38)	147(19)	189(16)	140(18)	-15(16)	-8(16)	-59(13)
C(39)	181(18)	214(17)	130(20)	40(14)	15(17)	-28(13)
C(40)	194(19)	250(19)	200(20)	44(15)	14(18)	35(14)
C(41)	148(19)	360(20)	260(20)	-5(17)	-20(18)	-21(16)
C(42)	230(20)	240(20)	390(30)	-58(17)	10(20)	-113(15)
C(43)	193(18)	118(17)	330(20)	-14(15)	38(19)	23(13)
C(44)	110(16)	113(16)	160(20)	-14(14)	13(15)	-49(12)
C(45)	183(18)	179(17)	160(20)	9(15)	8(16)	-38(13)
C(46)	173(19)	175(18)	260(20)	-39(15)	12(18)	19(13)
C(47)	189(19)	194(19)	290(20)	60(16)	-38(19)	-1(14)

C(48)	260(20)	247(19)	160(20)	32(16)	-47(18)	-65(15)
C(49)	186(18)	168(17)	170(20)	-24(15)	39(17)	-64(13)
C(50)	211(18)	93(16)	88(19)	23(13)	-11(16)	-57(13)
C(51)	240(20)	108(17)	210(20)	-5(15)	16(19)	2(13)
C(52)	280(20)	189(18)	170(20)	34(15)	-25(19)	-1(14)
C(53)	340(20)	250(20)	100(20)	-8(15)	29(19)	-83(16)
C(54)	250(20)	204(18)	180(20)	-18(15)	64(19)	-49(14)
C(55)	188(18)	139(17)	200(20)	22(14)	24(17)	-33(13)
C(56)	183(16)	140(17)	117(18)	-11(14)	-2(15)	29(13)
C(57)	223(18)	115(17)	140(20)	63(13)	-4(17)	33(12)
C(58)	250(20)	221(18)	210(20)	49(15)	65(18)	79(14)
C(59)	380(20)	172(18)	160(20)	-22(15)	-23(19)	124(15)
C(60)	300(20)	133(17)	230(20)	-41(15)	-37(19)	24(14)
C(61)	188(19)	168(17)	240(20)	33(15)	9(18)	-25(13)
C(62)	116(16)	119(16)	200(20)	38(14)	16(16)	-12(12)
C(63)	164(18)	163(17)	290(20)	15(15)	58(18)	-40(13)
C(64)	155(19)	183(19)	460(30)	42(18)	40(20)	28(14)
C(65)	144(19)	260(20)	450(30)	79(19)	-50(20)	-14(15)
C(66)	230(20)	240(20)	260(20)	17(16)	-54(19)	-79(15)
C(67)	192(19)	150(18)	230(20)	49(15)	7(18)	-39(13)
C(68)	182(17)	99(17)	156(19)	2(13)	10(16)	-36(12)
C(69)	168(18)	158(17)	210(20)	15(14)	15(17)	-17(12)
C(70)	270(20)	164(18)	240(20)	58(15)	3(19)	4(14)
C(71)	320(20)	237(19)	220(20)	89(16)	63(19)	-37(15)
C(72)	260(20)	270(20)	230(20)	11(16)	115(19)	-94(15)
C(73)	186(16)	166(17)	196(19)	-10(16)	0(16)	0(14)
C(74)	194(18)	140(17)	170(20)	4(14)	23(17)	-8(13)

ONO^{tBu})Ir(PPh$_3$)$_2$I, 13

Crystals were mounted on a glass fiber using Paratone oil, then placed on the diffractometer under a nitrogen stream at 100K.

The crystal contains pentane as a solvent of crystallization, two molecules per unit cell. Both were restrained to be similar and C91-C95 was restrained to approximate isotropic behavior. The tertiary butyl group on the pyridine ring, C26-C29, is disordered and both orientations were refined without restraint but constrained to have a total occupancy of unity.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S42. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **13**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ir(1)	3113(1)	519(1)	2138(1)	16(1)	1
I(2)	2769(1)	-542(1)	2743(1)	23(1)	1
P(1)	4725(1)	570(1)	2577(1)	18(1)	1
P(2)	1504(1)	499(1)	1694(1)	17(1)	1
O(1)	3013(2)	1218(1)	2722(1)	18(1)	1
O(2)	3212(2)	-154(1)	1542(1)	17(1)	1
N(1)	3393(2)	1320(1)	1685(1)	15(1)	1
C(1)	2503(3)	1762(2)	2611(1)	19(1)	1
C(2)	2076(3)	2094(2)	3006(1)	17(1)	1
C(3)	1384(3)	2577(2)	2856(1)	20(1)	1
C(4)	1121(3)	2812(2)	2344(1)	17(1)	1

C(5)	1649(3)	2578(2)	1991(1)	16(1)	1
C(6)	2354(3)	2071(2)	2115(1)	15(1)	1
C(7)	2993(3)	1944(2)	1738(1)	14(1)	1
C(8)	3236(3)	2497(2)	1451(1)	16(1)	1
C(9)	3818(3)	2426(2)	1086(1)	17(1)	1
C(10)	4168(3)	1767(2)	1028(1)	17(1)	1
C(11)	3980(3)	1219(2)	1335(1)	15(1)	1
C(12)	4393(3)	541(2)	1248(1)	16(1)	1
C(13)	5264(3)	534(2)	1069(1)	17(1)	1
C(14)	5647(3)	-55(2)	900(1)	18(1)	1
C(15)	5069(3)	-650(2)	860(1)	19(1)	1
C(16)	4217(3)	-682(2)	1024(1)	18(1)	1
C(17)	3915(3)	-91(2)	1281(1)	15(1)	1
C(18)	2422(3)	1953(2)	3576(1)	19(1)	1
C(19)	2324(3)	1188(2)	3727(1)	24(1)	1
C(20)	3461(3)	2163(2)	3695(2)	27(1)	1
C(21)	1885(3)	2376(2)	3927(2)	28(1)	1
C(22)	285(3)	3308(2)	2215(2)	24(1)	1
C(23)	-616(3)	2921(2)	2286(2)	32(1)	1
C(24)	179(3)	3575(2)	1664(2)	34(1)	1
C(25)	426(3)	3929(2)	2581(2)	30(1)	1
C(26)	4060(3)	3036(2)	762(2)	22(1)	1
C(27A)	4658(8)	3537(4)	1116(3)	43(3)	0.521(9)
C(28A)	4606(9)	2804(4)	335(4)	47(4)	0.521(9)
C(29A)	3174(7)	3375(5)	502(4)	46(3)	0.521(9)
C(27B)	3711(11)	3724(5)	945(5)	67(6)	0.479(9)
C(28B)	3554(10)	2939(6)	217(4)	53(4)	0.479(9)
C(29B)	5107(8)	3081(5)	784(5)	48(4)	0.479(9)
C(30)	6625(3)	-101(2)	757(1)	20(1)	1

C(31)	7106(3)	605(2)	786(1)	23(1)	1
C(32)	6563(3)	-372(2)	202(2)	29(1)	1
C(33)	7229(3)	-600(2)	1130(2)	31(1)	1
C(34)	3579(3)	-1323(2)	915(1)	20(1)	1
C(35)	3444(3)	-1696(2)	1415(2)	25(1)	1
C(36)	2641(3)	-1106(2)	617(1)	22(1)	1
C(37)	4008(3)	-1850(2)	582(2)	27(1)	1
C(38)	4952(3)	742(2)	3278(2)	24(1)	1
C(39)	5622(4)	1232(2)	3487(2)	40(1)	1
C(40)	5856(4)	1309(2)	4015(2)	50(2)	1
C(41)	5431(4)	927(3)	4343(2)	54(2)	1
C(42)	4779(4)	438(3)	4146(2)	54(2)	1
C(43)	4546(4)	350(3)	3612(2)	45(1)	1
C(44)	5491(3)	-176(2)	2553(1)	20(1)	1
C(45)	6408(3)	-178(2)	2825(2)	26(1)	1
C(46)	7007(3)	-712(2)	2770(2)	29(1)	1
C(47)	6701(3)	-1260(2)	2443(2)	26(1)	1
C(48)	5798(3)	-1270(2)	2185(2)	23(1)	1
C(49)	5182(3)	-734(2)	2241(1)	22(1)	1
C(50)	5389(3)	1283(2)	2353(1)	19(1)	1
C(51)	5066(3)	1952(2)	2408(1)	21(1)	1
C(52)	5572(3)	2519(2)	2270(1)	24(1)	1
C(53)	6395(3)	2423(2)	2080(2)	26(1)	1
C(54)	6719(3)	1760(2)	2022(2)	26(1)	1
C(55)	6216(3)	1196(2)	2154(2)	22(1)	1
C(56)	549(3)	647(2)	2061(1)	18(1)	1
C(57)	744(3)	752(2)	2589(2)	22(1)	1
C(58)	8(3)	842(2)	2867(2)	29(1)	1
C(59)	-910(3)	810(2)	2627(2)	30(1)	1

C(60)	-1110(3)	687(2)	2104(2)	28(1)	1
C(61)	-384(3)	609(2)	1826(2)	24(1)	1
C(62)	1050(3)	-289(2)	1336(1)	19(1)	1
C(63)	1194(3)	-939(2)	1562(2)	22(1)	1
C(64)	788(3)	-1514(2)	1312(2)	29(1)	1
C(65)	219(3)	-1460(2)	838(2)	34(1)	1
C(66)	67(3)	-821(2)	614(2)	33(1)	1
C(67)	483(3)	-235(2)	864(2)	28(1)	1
C(68)	1305(3)	1121(2)	1163(1)	19(1)	1
C(69)	634(3)	1639(2)	1121(1)	23(1)	1
C(70)	536(3)	2095(2)	705(2)	27(1)	1
C(71)	1121(3)	2049(2)	343(2)	27(1)	1
C(72)	1783(3)	1527(2)	377(1)	25(1)	1
C(73)	1875(3)	1060(2)	782(1)	21(1)	1
C(81)	2155(5)	7372(2)	4235(2)	73(2)	1
C(82)	2105(5)	8124(3)	4439(3)	99(3)	1
C(83)	2413(6)	8663(3)	4128(3)	108(3)	1
C(84)	2161(8)	9413(3)	4256(2)	150(5)	1
C(85)	2562(5)	9670(3)	4699(2)	142(4)	1
C(91)	-923(5)	9152(3)	4575(2)	155(4)	1
C(92)	-530(7)	9116(7)	5162(3)	239(7)	1
C(93)	313(7)	8713(5)	5312(4)	206(6)	1
C(94)	907(8)	8877(6)	5842(4)	203(5)	1
C(95)	1589(8)	8451(6)	6022(4)	227(6)	1

Table S43. Selected bond lengths [Å] and angles [°] for **13**.

Ir(1)-N(1)	2.040(3)	N(1)-Ir(1)-O(2)	89.52(10)
Ir(1)-O(2)	2.066(2)	N(1)-Ir(1)-O(1)	88.88(10)
Ir(1)-O(1)	2.076(2)	O(2)-Ir(1)-O(1)	178.36(9)
Ir(1)-P(2)	2.4233(10)	N(1)-Ir(1)-P(2)	89.69(9)
Ir(1)-P(1)	2.4247(11)	O(2)-Ir(1)-P(2)	78.59(8)
Ir(1)-I(2)	2.7013(3)	O(1)-Ir(1)-P(2)	101.03(8)
		N(1)-Ir(1)-P(1)	89.04(9)
		O(2)-Ir(1)-P(1)	102.10(8)
		O(1)-Ir(1)-P(1)	78.25(8)
		P(2)-Ir(1)-P(1)	178.55(3)
		N(1)-Ir(1)-I(2)	179.19(9)
		O(2)-Ir(1)-I(2)	90.56(6)
		O(1)-Ir(1)-I(2)	91.05(7)
		P(2)-Ir(1)-I(2)	91.12(2)
		P(1)-Ir(1)-I(2)	90.15(2)

Table S44. Bond lengths [Å] and angles [°] for **13**.

Ir(1)-N(1)	2.040(3)	C(9)-C(10)	1.394(5)
Ir(1)-O(2)	2.066(2)	C(9)-C(26)	1.533(5)
Ir(1)-O(1)	2.076(2)	C(10)-C(11)	1.389(5)
Ir(1)-P(2)	2.4233(10)	C(11)-C(12)	1.479(5)
Ir(1)-P(1)	2.4247(11)	C(12)-C(13)	1.411(5)
Ir(1)-I(2)	2.7013(3)	C(12)-C(17)	1.419(5)
P(1)-C(44)	1.828(4)	C(13)-C(14)	1.377(5)
P(1)-C(50)	1.837(4)	C(14)-C(15)	1.418(5)
P(1)-C(38)	1.854(4)	C(14)-C(30)	1.520(5)
P(2)-C(56)	1.830(4)	C(15)-C(16)	1.370(5)
P(2)-C(68)	1.836(4)	C(16)-C(17)	1.437(5)
P(2)-C(62)	1.861(4)	C(16)-C(34)	1.546(5)
O(1)-C(1)	1.293(5)	C(18)-C(21)	1.538(5)
O(2)-C(17)	1.320(4)	C(18)-C(20)	1.537(6)
N(1)-C(7)	1.360(4)	C(18)-C(19)	1.551(5)
N(1)-C(11)	1.365(5)	C(22)-C(24)	1.527(5)
C(1)-C(6)	1.424(5)	C(22)-C(23)	1.539(6)
C(1)-C(2)	1.445(5)	C(22)-C(25)	1.536(5)
C(2)-C(3)	1.380(5)	C(26)-C(29A)	1.500(10)
C(2)-C(18)	1.528(5)	C(26)-C(29B)	1.505(11)
C(3)-C(4)	1.417(5)	C(26)-C(28B)	1.516(11)
C(4)-C(5)	1.375(5)	C(26)-C(27A)	1.516(9)
C(4)-C(22)	1.537(5)	C(26)-C(27B)	1.531(10)
C(5)-C(6)	1.416(5)	C(26)-C(28A)	1.543(9)
C(6)-C(7)	1.481(5)	C(30)-C(31)	1.534(5)
C(7)-C(8)	1.392(5)	C(30)-C(32)	1.546(5)
C(8)-C(9)	1.384(5)	C(30)-C(33)	1.545(5)

C(34)-C(36)	1.510(6)	C(63)-C(64)	1.379(5)
C(34)-C(37)	1.543(5)	C(64)-C(65)	1.384(6)
C(34)-C(35)	1.546(5)	C(65)-C(66)	1.376(6)
C(38)-C(43)	1.367(6)	C(66)-C(67)	1.401(5)
C(38)-C(39)	1.403(6)	C(68)-C(69)	1.387(5)
C(39)-C(40)	1.385(6)	C(68)-C(73)	1.403(5)
C(40)-C(41)	1.358(7)	C(69)-C(70)	1.401(5)
C(41)-C(42)	1.378(7)	C(70)-C(71)	1.376(6)
C(42)-C(43)	1.403(6)	C(71)-C(72)	1.386(6)
C(44)-C(49)	1.390(5)	C(72)-C(73)	1.391(5)
C(44)-C(45)	1.398(6)	C(81)-C(82)	1.562(7)
C(45)-C(46)	1.374(5)	C(82)-C(83)	1.445(7)
C(46)-C(47)	1.394(5)	C(83)-C(84)	1.550(8)
C(47)-C(48)	1.369(6)	C(84)-C(85)	1.315(7)
C(48)-C(49)	1.391(5)	C(91)-C(92)	1.562(7)
C(50)-C(55)	1.388(6)	C(92)-C(93)	1.445(7)
C(50)-C(51)	1.396(5)	C(93)-C(94)	1.549(8)
C(51)-C(52)	1.402(5)	C(94)-C(95)	1.314(7)
C(52)-C(53)	1.375(6)		
C(53)-C(54)	1.385(5)	N(1)-Ir(1)-O(2)	89.52(10)
C(54)-C(55)	1.388(5)	N(1)-Ir(1)-O(1)	88.88(10)
C(56)-C(61)	1.389(6)	O(2)-Ir(1)-O(1)	178.36(9)
C(56)-C(57)	1.389(5)	N(1)-Ir(1)-P(2)	89.69(9)
C(57)-C(58)	1.397(6)	O(2)-Ir(1)-P(2)	78.59(8)
C(58)-C(59)	1.373(6)	O(1)-Ir(1)-P(2)	101.03(8)
C(59)-C(60)	1.384(6)	N(1)-Ir(1)-P(1)	89.04(9)
C(60)-C(61)	1.380(6)	O(2)-Ir(1)-P(1)	102.10(8)
C(62)-C(67)	1.378(5)	O(1)-Ir(1)-P(1)	78.25(8)
C(62)-C(63)	1.397(5)	P(2)-Ir(1)-P(1)	178.55(3)

N(1)-Ir(1)-I(2)	179.19(9)	C(5)-C(4)-C(3)	116.6(3)
O(2)-Ir(1)-I(2)	90.56(6)	C(5)-C(4)-C(22)	123.9(3)
O(1)-Ir(1)-I(2)	91.05(7)	C(3)-C(4)-C(22)	119.5(3)
P(2)-Ir(1)-I(2)	91.12(2)	C(4)-C(5)-C(6)	122.1(3)
P(1)-Ir(1)-I(2)	90.15(2)	C(5)-C(6)-C(1)	120.0(3)
C(44)-P(1)-C(50)	103.64(18)	C(5)-C(6)-C(7)	117.6(3)
C(44)-P(1)-C(38)	99.64(17)	C(1)-C(6)-C(7)	122.0(3)
C(50)-P(1)-C(38)	99.64(18)	N(1)-C(7)-C(8)	119.0(3)
C(44)-P(1)-Ir(1)	119.33(14)	N(1)-C(7)-C(6)	122.5(3)
C(50)-P(1)-Ir(1)	112.76(13)	C(8)-C(7)-C(6)	118.4(3)
C(38)-P(1)-Ir(1)	118.92(15)	C(9)-C(8)-C(7)	122.4(3)
C(56)-P(2)-C(68)	105.20(18)	C(8)-C(9)-C(10)	116.1(3)
C(56)-P(2)-C(62)	99.47(17)	C(8)-C(9)-C(26)	122.0(3)
C(68)-P(2)-C(62)	98.89(17)	C(10)-C(9)-C(26)	122.0(3)
C(56)-P(2)-Ir(1)	119.14(13)	C(11)-C(10)-C(9)	122.1(3)
C(68)-P(2)-Ir(1)	112.10(13)	N(1)-C(11)-C(10)	119.1(3)
C(62)-P(2)-Ir(1)	119.23(14)	N(1)-C(11)-C(12)	122.9(3)
C(1)-O(1)-Ir(1)	118.2(2)	C(10)-C(11)-C(12)	118.0(3)
C(17)-O(2)-Ir(1)	119.5(2)	C(13)-C(12)-C(17)	118.8(3)
C(7)-N(1)-C(11)	121.1(3)	C(13)-C(12)-C(11)	117.6(3)
C(7)-N(1)-Ir(1)	119.4(2)	C(17)-C(12)-C(11)	123.3(3)
C(11)-N(1)-Ir(1)	119.4(2)	C(14)-C(13)-C(12)	122.8(3)
O(1)-C(1)-C(6)	123.1(3)	C(13)-C(14)-C(15)	116.0(4)
O(1)-C(1)-C(2)	119.7(3)	C(13)-C(14)-C(30)	124.5(3)
C(6)-C(1)-C(2)	117.2(3)	C(15)-C(14)-C(30)	119.4(3)
C(3)-C(2)-C(1)	118.0(3)	C(16)-C(15)-C(14)	124.2(3)
C(3)-C(2)-C(18)	120.6(3)	C(15)-C(16)-C(17)	118.0(3)
C(1)-C(2)-C(18)	121.3(3)	C(15)-C(16)-C(34)	121.1(3)
C(2)-C(3)-C(4)	124.2(4)	C(17)-C(16)-C(34)	120.9(3)

O(2)-C(17)-C(12)	122.4(3)	C(9)-C(26)-C(27B)	112.5(4)
O(2)-C(17)-C(16)	119.3(3)	C(29A)-C(26)-C(28A)	107.0(6)
C(12)-C(17)-C(16)	118.3(3)	C(29B)-C(26)-C(28A)	54.3(6)
C(21)-C(18)-C(2)	112.4(3)	C(28B)-C(26)-C(28A)	59.7(6)
C(21)-C(18)-C(20)	107.8(3)	C(27A)-C(26)-C(28A)	109.2(7)
C(2)-C(18)-C(20)	107.7(3)	C(9)-C(26)-C(28A)	111.7(4)
C(21)-C(18)-C(19)	106.3(3)	C(27B)-C(26)-C(28A)	135.8(5)
C(2)-C(18)-C(19)	113.3(3)	C(14)-C(30)-C(31)	111.4(3)
C(20)-C(18)-C(19)	109.1(3)	C(14)-C(30)-C(32)	109.9(3)
C(24)-C(22)-C(4)	112.2(3)	C(31)-C(30)-C(32)	107.9(3)
C(24)-C(22)-C(23)	109.0(4)	C(14)-C(30)-C(33)	109.3(3)
C(4)-C(22)-C(23)	108.3(3)	C(31)-C(30)-C(33)	109.0(3)
C(24)-C(22)-C(25)	108.3(3)	C(32)-C(30)-C(33)	109.3(3)
C(4)-C(22)-C(25)	109.4(3)	C(36)-C(34)-C(37)	107.3(3)
C(23)-C(22)-C(25)	109.6(3)	C(36)-C(34)-C(35)	110.4(3)
C(29A)-C(26)-C(29B)	140.1(6)	C(37)-C(34)-C(35)	107.1(3)
C(29A)-C(26)-C(28B)	51.5(6)	C(36)-C(34)-C(16)	109.1(3)
C(29B)-C(26)-C(28B)	111.6(8)	C(37)-C(34)-C(16)	111.0(3)
C(29A)-C(26)-C(27A)	110.9(6)	C(35)-C(34)-C(16)	111.8(3)
C(29B)-C(26)-C(27A)	58.1(6)	C(43)-C(38)-C(39)	117.6(4)
C(28B)-C(26)-C(27A)	143.3(5)	C(43)-C(38)-P(1)	121.1(3)
C(29A)-C(26)-C(9)	109.9(5)	C(39)-C(38)-P(1)	120.9(3)
C(29B)-C(26)-C(9)	109.9(5)	C(40)-C(39)-C(38)	120.5(5)
C(28B)-C(26)-C(9)	108.4(5)	C(41)-C(40)-C(39)	121.3(5)
C(27A)-C(26)-C(9)	108.1(4)	C(40)-C(41)-C(42)	119.1(5)
C(29A)-C(26)-C(27B)	57.5(7)	C(41)-C(42)-C(43)	120.0(5)
C(29B)-C(26)-C(27B)	108.5(8)	C(38)-C(43)-C(42)	121.4(5)
C(28B)-C(26)-C(27B)	105.9(8)	C(49)-C(44)-C(45)	119.2(4)
C(27A)-C(26)-C(27B)	55.3(7)	C(49)-C(44)-P(1)	120.0(3)

C(45)-C(44)-P(1)	120.8(3)	C(62)-C(67)-C(66)	120.6(4)
C(46)-C(45)-C(44)	120.5(4)	C(69)-C(68)-C(73)	119.1(3)
C(45)-C(46)-C(47)	120.0(4)	C(69)-C(68)-P(2)	123.9(3)
C(48)-C(47)-C(46)	119.9(4)	C(73)-C(68)-P(2)	117.0(3)
C(47)-C(48)-C(49)	120.6(4)	C(68)-C(69)-C(70)	120.2(4)
C(48)-C(49)-C(44)	119.8(4)	C(71)-C(70)-C(69)	120.5(4)
C(55)-C(50)-C(51)	118.4(4)	C(70)-C(71)-C(72)	119.7(4)
C(55)-C(50)-P(1)	123.7(3)	C(71)-C(72)-C(73)	120.4(4)
C(51)-C(50)-P(1)	117.8(3)	C(72)-C(73)-C(68)	120.0(4)
C(50)-C(51)-C(52)	120.4(4)	C(83)-C(82)-C(81)	116.5(6)
C(53)-C(52)-C(51)	120.3(4)	C(82)-C(83)-C(84)	116.9(6)
C(52)-C(53)-C(54)	119.5(4)	C(85)-C(84)-C(83)	117.8(7)
C(53)-C(54)-C(55)	120.4(4)	C(93)-C(92)-C(91)	116.7(6)
C(54)-C(55)-C(50)	121.0(4)	C(92)-C(93)-C(94)	116.9(6)
C(61)-C(56)-C(57)	118.6(4)	C(95)-C(94)-C(93)	117.9(7)
C(61)-C(56)-P(2)	120.9(3)		
C(57)-C(56)-P(2)	120.3(3)		
C(56)-C(57)-C(58)	119.8(4)		
C(59)-C(58)-C(57)	120.7(4)		
C(58)-C(59)-C(60)	119.8(4)		
C(61)-C(60)-C(59)	119.6(4)		
C(60)-C(61)-C(56)	121.4(4)		
C(67)-C(62)-C(63)	118.7(3)		
C(67)-C(62)-P(2)	120.3(3)		
C(63)-C(62)-P(2)	120.6(3)		
C(64)-C(63)-C(62)	120.3(4)		
C(65)-C(64)-C(63)	121.0(4)		
C(64)-C(65)-C(66)	119.1(4)		
C(65)-C(66)-C(67)	120.3(4)		

Table S45. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **13**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	231(1)	112(1)	157(1)	-9(1)	84(1)	5(1)
I(2)	336(2)	178(1)	196(1)	19(1)	75(1)	-35(1)
P(1)	232(6)	146(5)	178(5)	-19(4)	59(4)	38(5)
P(2)	214(6)	158(4)	160(4)	-12(4)	59(4)	-18(5)
O(1)	267(17)	166(13)	133(12)	-9(10)	69(12)	11(12)
O(2)	267(17)	85(12)	188(13)	-28(10)	104(13)	-33(11)
N(1)	147(18)	174(15)	122(15)	-59(12)	34(14)	4(13)
C(1)	190(20)	200(20)	200(19)	-132(15)	87(18)	-132(17)
C(2)	210(20)	93(17)	220(20)	-7(14)	81(18)	-23(15)
C(3)	210(20)	157(19)	250(20)	-67(15)	86(19)	-14(16)
C(4)	190(20)	77(17)	250(20)	6(15)	39(18)	-5(15)
C(5)	170(20)	123(17)	207(19)	-8(14)	40(17)	-26(15)
C(6)	160(20)	132(17)	180(18)	-39(14)	48(17)	-23(15)
C(7)	150(20)	125(17)	155(18)	-40(14)	17(16)	-4(15)
C(8)	200(20)	86(17)	205(19)	4(14)	34(18)	14(15)
C(9)	200(20)	142(18)	165(18)	7(14)	14(18)	-24(16)
C(10)	190(20)	220(20)	123(18)	-10(15)	66(17)	-23(16)
C(11)	150(20)	152(18)	153(18)	-43(14)	37(17)	-8(16)
C(12)	220(20)	124(16)	133(16)	-20(15)	62(15)	-4(18)
C(13)	220(20)	156(16)	129(16)	4(16)	38(16)	-22(18)
C(14)	220(20)	159(18)	149(18)	0(14)	42(17)	27(16)
C(15)	270(20)	126(19)	182(18)	-10(14)	69(18)	10(16)
C(16)	250(20)	99(18)	191(19)	-7(14)	61(18)	-14(15)
C(17)	190(20)	148(18)	112(17)	19(14)	33(17)	5(16)

C(18)	250(20)	138(18)	199(19)	-35(15)	89(19)	2(16)
C(19)	300(30)	220(20)	200(20)	33(16)	63(19)	0(18)
C(20)	340(30)	280(20)	190(20)	-51(17)	60(20)	-60(20)
C(21)	420(30)	220(20)	240(20)	-25(17)	170(20)	51(19)
C(22)	220(30)	210(20)	290(20)	-7(17)	80(20)	79(18)
C(23)	250(30)	290(20)	420(30)	-60(20)	80(20)	40(20)
C(24)	340(30)	370(30)	320(20)	20(20)	30(20)	170(20)
C(25)	300(30)	210(20)	390(30)	-35(18)	90(20)	84(19)
C(26)	310(30)	139(18)	230(20)	43(15)	120(20)	7(17)
C(27A)	680(90)	250(50)	390(50)	60(40)	160(60)	-230(50)
C(28A)	850(100)	180(40)	510(70)	100(40)	460(70)	50(50)
C(29A)	430(70)	420(60)	500(70)	270(60)	40(50)	30(50)
C(27B)	1190(150)	290(60)	750(90)	260(60)	810(110)	260(70)
C(28B)	650(100)	560(70)	340(60)	280(50)	-40(60)	-280(70)
C(29B)	350(70)	370(60)	760(90)	330(60)	160(60)	-40(50)
C(30)	240(20)	139(18)	220(20)	-11(15)	73(19)	10(16)
C(31)	230(20)	210(20)	260(20)	-11(17)	95(18)	-7(18)
C(32)	360(30)	210(20)	340(20)	-72(17)	210(20)	-24(18)
C(33)	260(30)	220(20)	450(30)	98(19)	90(20)	30(19)
C(34)	240(20)	120(18)	240(20)	-29(15)	85(19)	-4(16)
C(35)	340(30)	139(19)	290(20)	-14(16)	90(20)	-47(18)
C(36)	300(30)	169(19)	210(20)	-52(15)	91(19)	-61(17)
C(37)	340(30)	170(20)	320(20)	-73(17)	100(20)	-27(18)
C(38)	290(30)	220(20)	200(20)	-48(16)	30(20)	102(18)
C(39)	600(40)	260(20)	310(20)	-64(19)	-50(30)	20(20)
C(40)	740(50)	360(30)	350(30)	-120(20)	-90(30)	20(30)
C(41)	530(40)	770(40)	290(30)	-220(30)	-30(30)	250(30)
C(42)	420(40)	940(40)	280(30)	150(30)	80(30)	50(30)
C(43)	340(30)	720(40)	260(20)	10(20)	10(20)	-90(30)

C(44)	290(30)	146(18)	181(19)	31(15)	79(19)	57(17)
C(45)	310(30)	147(19)	310(20)	-14(17)	40(20)	20(18)
C(46)	250(30)	310(20)	310(20)	97(18)	30(20)	69(19)
C(47)	340(30)	152(19)	300(20)	60(17)	130(20)	75(18)
C(48)	370(30)	116(18)	240(20)	31(15)	120(20)	48(18)
C(49)	310(30)	187(19)	165(19)	56(15)	61(19)	40(17)
C(50)	220(20)	176(19)	169(19)	-24(15)	4(18)	-3(17)
C(51)	240(20)	177(19)	190(20)	-41(16)	14(19)	30(17)
C(52)	320(30)	126(19)	260(20)	-29(16)	10(20)	26(18)
C(53)	310(30)	170(20)	280(20)	-9(16)	40(20)	-45(18)
C(54)	220(30)	250(20)	340(20)	-15(18)	90(20)	16(18)
C(55)	220(20)	186(19)	270(20)	-34(16)	15(19)	28(17)
C(56)	260(20)	62(18)	234(19)	7(14)	89(18)	-7(15)
C(57)	230(20)	158(18)	280(20)	-45(16)	70(20)	-40(17)
C(58)	310(30)	290(20)	300(20)	-86(18)	100(20)	-70(20)
C(59)	300(30)	250(20)	390(30)	-51(19)	170(20)	2(19)
C(60)	220(30)	260(20)	380(30)	-21(18)	70(20)	8(18)
C(61)	290(30)	180(20)	260(20)	23(16)	69(19)	34(18)
C(62)	220(20)	167(18)	189(19)	-47(15)	82(19)	-59(16)
C(63)	270(30)	200(20)	210(20)	-28(16)	98(19)	-46(18)
C(64)	410(30)	220(20)	260(20)	-44(17)	130(20)	-110(20)
C(65)	420(30)	300(20)	300(20)	-90(19)	110(20)	-190(20)
C(66)	340(30)	360(20)	250(20)	-31(19)	-10(20)	-110(20)
C(67)	290(30)	270(20)	280(20)	-27(18)	30(20)	-43(19)
C(68)	230(20)	168(19)	167(19)	-23(15)	10(18)	-75(17)
C(69)	260(30)	220(20)	210(20)	-21(16)	41(19)	-30(18)
C(70)	300(30)	190(20)	280(20)	-4(17)	-50(20)	-6(19)
C(71)	390(30)	220(20)	180(20)	2(16)	0(20)	-80(20)
C(72)	320(30)	270(20)	159(19)	-29(16)	28(19)	-100(20)

C(73)	200(20)	210(20)	210(20)	-37(16)	7(18)	-45(17)
C(81)	880(60)	450(30)	890(50)	120(30)	240(40)	300(30)
C(82)	830(60)	1220(60)	960(60)	290(50)	210(50)	450(50)
C(83)	830(70)	980(60)	1500(80)	450(60)	440(60)	0(50)
C(84)	3170(160)	750(50)	630(50)	-170(40)	440(70)	-950(80)
C(85)	1180(90)	1490(90)	1730(90)	970(70)	690(80)	300(70)
C(91)	1280(70)	1690(70)	1740(70)	-580(60)	440(60)	-330(60)
C(92)	2580(110)	2360(100)	2400(100)	410(80)	920(80)	410(80)
C(93)	1620(90)	2390(90)	2290(90)	-390(80)	730(80)	90(70)
C(94)	2370(100)	2600(90)	1230(70)	-40(70)	610(70)	900(80)
C(95)	2280(100)	2340(100)	2350(100)	-270(80)	890(80)	140(80)

(ONO^{tBu})Ir(PEt_3)$_2$Me, 14.

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S46. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **14**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	1095(1)	935(1)	2083(1)	10(1)
P(1)	1164(1)	886(1)	37(1)	13(1)
P(2)	1008(1)	920(1)	4130(1)	12(1)
O(1)	2649(1)	709(1)	2090(1)	12(1)
O(2)	-437(1)	1175(1)	2104(1)	13(1)
N(1)	1761(1)	1483(1)	2075(1)	10(1)
C(1)	3434(1)	858(1)	2790(2)	12(1)
C(2)	4330(1)	624(1)	3212(2)	12(1)
C(3)	5034(1)	759(1)	4116(2)	14(1)
C(4)	4949(1)	1122(1)	4613(2)	13(1)
C(5)	4175(1)	1357(1)	4081(2)	13(1)
C(6)	3442(1)	1243(1)	3155(2)	11(1)
C(7)	2780(1)	1548(1)	2564(2)	12(1)
C(8)	3240(1)	1911(1)	2520(2)	13(1)
C(9)	2643(1)	2217(1)	2084(2)	12(1)
C(10)	1586(1)	2141(1)	1625(2)	12(1)
C(11)	1172(1)	1775(1)	1570(2)	11(1)
C(12)	77(1)	1714(1)	966(2)	12(1)
C(13)	-215(1)	1953(1)	16(2)	13(1)
C(14)	-1261(1)	1964(1)	-515(2)	14(1)
C(15)	-2045(1)	1746(1)	17(2)	16(1)
C(16)	-1815(1)	1502(1)	946(2)	14(1)
C(17)	-695(1)	1453(1)	1361(2)	13(1)
C(18)	4502(1)	231(1)	2671(2)	14(1)

C(19)	4616(2)	270(1)	1350(2)	18(1)
C(20)	3541(2)	-35(1)	2889(2)	20(1)
C(21)	5545(2)	37(1)	3200(2)	19(1)
C(22)	5636(1)	1251(1)	5712(2)	16(1)
C(23)	4973(2)	1183(1)	6788(2)	26(1)
C(24)	5921(2)	1673(1)	5650(2)	22(1)
C(25)	6710(2)	1032(1)	5878(2)	20(1)
C(26)	3084(1)	2622(1)	2080(2)	14(1)
C(27)	3073(2)	2762(1)	812(2)	20(1)
C(28)	2354(2)	2878(1)	2777(2)	22(1)
C(29)	4257(1)	2648(1)	2630(2)	19(1)
C(30)	-1532(1)	2190(1)	-1647(2)	16(1)
C(31)	-2742(2)	2298(1)	-1785(2)	22(1)
C(32)	-1247(2)	1944(1)	-2693(2)	25(1)
C(33)	-876(2)	2558(1)	-1667(2)	25(1)
C(34)	-2734(1)	1313(1)	1585(2)	19(1)
C(35)	-2680(2)	1467(1)	2845(2)	24(1)
C(36)	-2660(2)	878(1)	1619(2)	25(1)
C(37)	-3875(2)	1411(1)	1026(2)	31(1)
C(38)	2083(2)	1217(1)	-648(2)	17(1)
C(39)	3298(2)	1183(1)	-274(2)	22(1)
C(40)	1666(2)	418(1)	-368(2)	16(1)
C(41)	1907(2)	357(1)	-1652(2)	22(1)
C(42)	-63(1)	954(1)	-949(2)	17(1)
C(43)	-956(2)	660(1)	-856(2)	26(1)
C(44)	1938(1)	603(1)	4996(2)	16(1)
C(45)	1599(2)	186(1)	4993(2)	22(1)
C(46)	-346(1)	784(1)	4566(2)	15(1)
C(47)	-506(2)	798(1)	5881(2)	20(1)

C(48)	1250(2)	1367(1)	4922(2)	17(1)
C(49)	412(2)	1676(1)	4604(2)	21(1)
C(50)	415(1)	385(1)	2041(2)	16(1)

Table S47. Selected bond lengths [Å] and angles [°] for **14**.

Ir(1)-O(2)	2.0674(11)	O(2)-Ir(1)-O(1)	178.26(5)
Ir(1)-O(1)	2.0702(11)	O(2)-Ir(1)-N(1)	88.65(5)
Ir(1)-N(1)	2.1050(14)	O(1)-Ir(1)-N(1)	89.83(5)
Ir(1)-C(50)	2.1154(17)	O(2)-Ir(1)-C(50)	91.12(6)
Ir(1)-P(2)	2.3479(5)	O(1)-Ir(1)-C(50)	90.42(6)
Ir(1)-P(1)	2.3514(5)	N(1)-Ir(1)-C(50)	178.40(6)
		O(2)-Ir(1)-P(2)	84.03(4)
		O(1)-Ir(1)-P(2)	95.23(4)
		N(1)-Ir(1)-P(2)	93.93(4)
		C(50)-Ir(1)-P(2)	87.61(5)
		O(2)-Ir(1)-P(1)	97.78(4)
		O(1)-Ir(1)-P(1)	83.10(4)
		N(1)-Ir(1)-P(1)	91.40(4)
		C(50)-Ir(1)-P(1)	87.07(5)
		P(2)-Ir(1)-P(1)	174.416(16)

Table S48. Bond lengths [Å] and angles [°] for **14.**

Ir(1)-O(2)	2.0674(11)	P(1)-C(38)	1.8384(18)
Ir(1)-O(1)	2.0702(11)	P(2)-C(46)	1.8327(18)
Ir(1)-N(1)	2.1050(14)	P(2)-C(48)	1.8355(18)
Ir(1)-C(50)	2.1154(17)	P(2)-C(44)	1.8424(17)
Ir(1)-P(2)	2.3479(5)	O(1)-C(1)	1.322(2)
Ir(1)-P(1)	2.3514(5)	O(2)-C(17)	1.322(2)
P(1)-C(40)	1.8353(18)	N(1)-C(7)	1.357(2)
P(1)-C(42)	1.8367(17)	N(1)-C(11)	1.365(2)

C(1)-C(6)	1.424(2)	C(26)-C(27)	1.531(2)
C(1)-C(2)	1.435(2)	C(26)-C(28)	1.536(2)
C(2)-C(3)	1.387(2)	C(26)-C(29)	1.536(2)
C(2)-C(18)	1.544(2)	C(30)-C(33)	1.533(2)
C(3)-C(4)	1.411(2)	C(30)-C(31)	1.534(2)
C(4)-C(5)	1.373(2)	C(30)-C(32)	1.538(3)
C(4)-C(22)	1.535(2)	C(34)-C(35)	1.537(3)
C(5)-C(6)	1.402(2)	C(34)-C(37)	1.541(2)
C(6)-C(7)	1.486(2)	C(34)-C(36)	1.542(3)
C(7)-C(8)	1.405(2)	C(38)-C(39)	1.529(2)
C(8)-C(9)	1.381(2)	C(40)-C(41)	1.531(2)
C(9)-C(10)	1.394(2)	C(42)-C(43)	1.519(3)
C(9)-C(26)	1.530(2)	C(44)-C(45)	1.533(2)
C(10)-C(11)	1.391(2)	C(46)-C(47)	1.529(2)
C(11)-C(12)	1.487(2)	C(48)-C(49)	1.528(2)
C(12)-C(13)	1.405(2)		
C(12)-C(17)	1.418(2)	O(2)-Ir(1)-O(1)	178.26(5)
C(13)-C(14)	1.385(2)	O(2)-Ir(1)-N(1)	88.65(5)
C(14)-C(15)	1.403(2)	O(1)-Ir(1)-N(1)	89.83(5)
C(14)-C(30)	1.538(2)	O(2)-Ir(1)-C(50)	91.12(6)
C(15)-C(16)	1.383(2)	O(1)-Ir(1)-C(50)	90.42(6)
C(16)-C(17)	1.435(2)	N(1)-Ir(1)-C(50)	178.40(6)
C(16)-C(34)	1.539(2)	O(2)-Ir(1)-P(2)	84.03(4)
C(18)-C(19)	1.531(2)	O(1)-Ir(1)-P(2)	95.23(4)
C(18)-C(21)	1.540(2)	N(1)-Ir(1)-P(2)	93.93(4)
C(18)-C(20)	1.541(2)	C(50)-Ir(1)-P(2)	87.61(5)
C(22)-C(25)	1.531(2)	O(2)-Ir(1)-P(1)	97.78(4)
C(22)-C(24)	1.534(2)	O(1)-Ir(1)-P(1)	83.10(4)
C(22)-C(23)	1.539(3)	N(1)-Ir(1)-P(1)	91.40(4)

C(50)-Ir(1)-P(1)	87.07(5)	C(4)-C(5)-C(6)	123.44(16)
P(2)-Ir(1)-P(1)	174.416(16)	C(5)-C(6)-C(1)	119.19(15)
C(40)-P(1)-C(42)	103.85(8)	C(5)-C(6)-C(7)	116.02(15)
C(40)-P(1)-C(38)	103.93(9)	C(1)-C(6)-C(7)	124.61(15)
C(42)-P(1)-C(38)	99.07(8)	N(1)-C(7)-C(8)	120.12(15)
C(40)-P(1)-Ir(1)	110.68(6)	N(1)-C(7)-C(6)	121.80(15)
C(42)-P(1)-Ir(1)	121.14(6)	C(8)-C(7)-C(6)	118.08(15)
C(38)-P(1)-Ir(1)	116.09(6)	C(9)-C(8)-C(7)	121.58(16)
C(46)-P(2)-C(48)	102.27(9)	C(8)-C(9)-C(10)	116.34(16)
C(46)-P(2)-C(44)	103.62(8)	C(8)-C(9)-C(26)	123.60(15)
C(48)-P(2)-C(44)	100.69(8)	C(10)-C(9)-C(26)	120.05(15)
C(46)-P(2)-Ir(1)	112.26(6)	C(11)-C(10)-C(9)	121.67(16)
C(48)-P(2)-Ir(1)	117.06(6)	N(1)-C(11)-C(10)	120.12(15)
C(44)-P(2)-Ir(1)	118.75(6)	N(1)-C(11)-C(12)	121.63(15)
C(1)-O(1)-Ir(1)	118.90(10)	C(10)-C(11)-C(12)	118.25(15)
C(17)-O(2)-Ir(1)	118.49(11)	C(13)-C(12)-C(17)	119.79(15)
C(7)-N(1)-C(11)	119.71(14)	C(13)-C(12)-C(11)	116.53(15)
C(7)-N(1)-Ir(1)	120.17(11)	C(17)-C(12)-C(11)	123.46(16)
C(11)-N(1)-Ir(1)	120.12(11)	C(14)-C(13)-C(12)	122.39(16)
O(1)-C(1)-C(6)	123.40(15)	C(13)-C(14)-C(15)	116.10(16)
O(1)-C(1)-C(2)	119.09(15)	C(13)-C(14)-C(30)	121.62(16)
C(6)-C(1)-C(2)	117.52(15)	C(15)-C(14)-C(30)	122.24(15)
C(3)-C(2)-C(1)	118.63(16)	C(16)-C(15)-C(14)	124.32(16)
C(3)-C(2)-C(18)	120.87(15)	C(15)-C(16)-C(17)	118.17(16)
C(1)-C(2)-C(18)	120.50(15)	C(15)-C(16)-C(34)	121.08(16)
C(2)-C(3)-C(4)	123.58(16)	C(17)-C(16)-C(34)	120.58(16)
C(5)-C(4)-C(3)	116.11(16)	O(2)-C(17)-C(12)	123.37(15)
C(5)-C(4)-C(22)	120.66(16)	O(2)-C(17)-C(16)	119.07(16)
C(3)-C(4)-C(22)	123.19(15)	C(12)-C(17)-C(16)	117.54(16)

C(19)-C(18)-C(21)	107.40(15)	C(37)-C(34)-C(36)	106.65(16)
C(19)-C(18)-C(20)	109.66(15)	C(39)-C(38)-P(1)	116.57(13)
C(21)-C(18)-C(20)	107.05(15)	C(41)-C(40)-P(1)	117.24(13)
C(19)-C(18)-C(2)	109.67(14)	C(43)-C(42)-P(1)	115.81(13)
C(21)-C(18)-C(2)	112.03(14)	C(45)-C(44)-P(2)	115.24(12)
C(20)-C(18)-C(2)	110.93(14)	C(47)-C(46)-P(2)	115.95(12)
C(25)-C(22)-C(24)	107.46(15)	C(49)-C(48)-P(2)	114.41(12)
C(25)-C(22)-C(4)	111.99(15)		
C(24)-C(22)-C(4)	111.46(15)		
C(25)-C(22)-C(23)	108.67(16)		
C(24)-C(22)-C(23)	108.87(16)		
C(4)-C(22)-C(23)	108.32(15)		
C(9)-C(26)-C(27)	109.01(14)		
C(9)-C(26)-C(28)	109.40(15)		
C(27)-C(26)-C(28)	109.24(15)		
C(9)-C(26)-C(29)	112.19(14)		
C(27)-C(26)-C(29)	108.41(15)		
C(28)-C(26)-C(29)	108.54(15)		
C(33)-C(30)-C(31)	107.19(15)		
C(33)-C(30)-C(32)	108.80(16)		
C(31)-C(30)-C(32)	109.22(15)		
C(33)-C(30)-C(14)	111.75(15)		
C(31)-C(30)-C(14)	111.69(15)		
C(32)-C(30)-C(14)	108.13(15)		
C(35)-C(34)-C(16)	107.57(15)		
C(35)-C(34)-C(37)	106.86(17)		
C(16)-C(34)-C(37)	112.45(16)		
C(35)-C(34)-C(36)	109.34(16)		
C(16)-C(34)-C(36)	113.73(16)		

Table S49. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **14**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	110(1)	91(1)	94(1)	2(1)	-5(1)	-15(1)
P(1)	155(2)	122(2)	105(2)	-2(2)	-4(2)	-11(2)
P(2)	125(2)	135(2)	104(2)	5(2)	-1(2)	0(2)
O(1)	117(6)	114(6)	136(7)	-25(5)	-10(5)	4(5)
O(2)	108(6)	141(6)	145(7)	33(5)	1(5)	2(5)
N(1)	114(7)	83(7)	114(8)	-13(6)	6(6)	-14(6)
C(1)	136(8)	133(9)	99(9)	8(7)	26(6)	-16(7)
C(2)	145(8)	115(9)	119(9)	13(7)	38(7)	-3(7)
C(3)	126(8)	144(9)	143(9)	29(7)	21(7)	24(7)
C(4)	115(8)	143(9)	121(9)	0(7)	10(7)	-11(7)
C(5)	138(8)	99(8)	142(9)	-15(7)	26(7)	-4(7)
C(6)	99(8)	121(9)	120(9)	8(7)	11(7)	-7(7)
C(7)	128(8)	114(9)	102(9)	-6(7)	8(7)	6(7)
C(8)	102(8)	154(9)	127(9)	-8(7)	-12(7)	-17(7)
C(9)	137(8)	100(8)	113(9)	-5(7)	25(7)	-11(7)
C(10)	133(8)	105(8)	132(9)	15(7)	-5(7)	26(7)
C(11)	112(8)	144(9)	87(9)	-3(7)	16(6)	-2(7)
C(12)	104(8)	115(9)	138(9)	-12(7)	-9(7)	1(7)
C(13)	124(8)	115(9)	146(9)	-8(7)	20(7)	-15(7)
C(14)	143(9)	128(9)	137(9)	-1(7)	-17(7)	5(7)
C(15)	113(8)	183(9)	176(10)	3(8)	-34(7)	-2(7)
C(16)	134(8)	160(9)	139(9)	0(7)	-5(7)	-34(7)
C(17)	142(8)	144(9)	103(9)	-23(7)	3(7)	0(7)
C(18)	150(9)	116(9)	157(10)	-5(7)	18(7)	28(7)

C(19)	204(9)	172(10)	175(10)	-29(8)	38(8)	18(8)
C(20)	210(9)	132(9)	245(11)	-13(8)	31(8)	2(8)
C(21)	210(10)	145(9)	206(11)	-8(8)	20(8)	45(8)
C(22)	163(9)	166(9)	145(10)	-16(8)	-29(7)	26(7)
C(23)	269(11)	351(12)	171(11)	-25(9)	-7(8)	11(9)
C(24)	187(9)	197(10)	248(11)	-60(9)	-90(8)	18(8)
C(25)	206(10)	177(10)	212(11)	-17(8)	-82(8)	18(8)
C(26)	143(8)	100(8)	169(10)	11(7)	-6(7)	-24(7)
C(27)	228(10)	167(10)	205(10)	43(8)	-16(8)	-52(8)
C(28)	239(10)	143(10)	286(12)	-59(8)	28(8)	-18(8)
C(29)	189(9)	141(9)	232(11)	33(8)	-46(8)	-52(8)
C(30)	145(9)	182(9)	150(10)	38(8)	-19(7)	-18(8)
C(31)	193(10)	259(11)	206(11)	63(9)	-33(8)	30(8)
C(32)	255(11)	335(12)	166(11)	14(9)	-14(8)	32(9)
C(33)	235(10)	237(11)	264(11)	115(9)	-64(8)	-42(9)
C(34)	129(9)	230(10)	212(11)	56(8)	-12(7)	-30(8)
C(35)	194(10)	262(11)	260(12)	50(9)	77(8)	-3(8)
C(36)	198(10)	252(11)	309(12)	28(9)	25(8)	-94(8)
C(37)	133(10)	449(14)	355(14)	164(11)	0(9)	-45(9)
C(38)	237(10)	154(9)	128(10)	22(8)	32(7)	-18(8)
C(39)	226(10)	257(11)	197(11)	23(9)	40(8)	-48(8)
C(40)	199(9)	161(9)	133(9)	-28(8)	-12(7)	13(8)
C(41)	304(11)	211(10)	164(10)	-40(8)	40(8)	27(9)
C(42)	201(9)	168(9)	126(9)	-21(8)	-44(7)	14(8)
C(43)	215(10)	283(11)	282(12)	-4(10)	-73(9)	-9(9)
C(44)	141(9)	212(10)	129(9)	47(8)	2(7)	14(7)
C(45)	216(10)	216(10)	214(11)	57(9)	12(8)	51(8)
C(46)	133(8)	181(9)	136(9)	21(8)	20(7)	7(7)
C(47)	183(9)	262(10)	158(10)	47(8)	34(8)	40(8)

C(48)	180(9)	187(10)	140(10)	-40(8)	12(7)	-23(8)
C(49)	279(11)	169(10)	192(11)	-38(8)	24(8)	18(8)
C(50)	186(9)	130(9)	169(10)	1(8)	4(7)	-47(7)

$(ONO^{tBu})Ir(PEt_3)_2I$, 15

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The crystal is a mixture of the methyl and iodine compounds. The ratio of methyl to iodine is 0.33:0.67. Restraints (ISOR) were placed on the methyl carbon to encourage the anisotropic displacement parameters to approximate isotropic behavior.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S50. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **15**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ir(1)	8944(1)	957(1)	7831(1)	10(1)	1
I(2)	9846(1)	279(1)	7876(1)	16(1)	0.665(1)
C(50)	9620(5)	403(2)	7944(5)	16(1)	0.335(1)
P(1)	9031(1)	931(1)	5770(1)	14(1)	1
P(2)	8862(1)	919(1)	9891(1)	13(1)	1
O(1)	10479(1)	1194(1)	7779(1)	14(1)	1
O(2)	7391(1)	734(1)	7860(1)	13(1)	1

N(1)	8288(1)	1489(1)	7812(1)	11(1)	1
C(1)	10745(1)	1467(1)	8518(1)	13(1)	1
C(2)	11867(1)	1520(1)	8918(1)	15(1)	1
C(3)	12097(1)	1761(1)	9854(2)	17(1)	1
C(4)	11302(1)	1974(1)	10393(1)	14(1)	1
C(5)	10255(1)	1962(1)	9872(1)	14(1)	1
C(6)	9964(1)	1724(1)	8920(1)	12(1)	1
C(7)	8871(1)	1779(1)	8318(1)	12(1)	1
C(8)	8448(1)	2141(1)	8268(1)	13(1)	1
C(9)	7392(1)	2213(1)	7796(1)	12(1)	1
C(10)	6802(1)	1910(1)	7347(1)	13(1)	1
C(11)	7271(1)	1552(1)	7316(1)	11(1)	1
C(12)	6607(1)	1249(1)	6744(1)	12(1)	1
C(13)	5878(1)	1356(1)	5803(1)	13(1)	1
C(14)	5108(1)	1117(1)	5288(1)	13(1)	1
C(15)	5016(1)	763(1)	5821(1)	14(1)	1
C(16)	5708(1)	637(1)	6743(1)	13(1)	1
C(17)	6609(1)	872(1)	7140(1)	12(1)	1
C(18)	12795(1)	1335(1)	8274(2)	20(1)	1
C(19)	12722(2)	1484(1)	7012(2)	25(1)	1
C(20)	12729(2)	906(1)	8260(2)	27(1)	1
C(21)	13936(1)	1441(1)	8805(2)	32(1)	1
C(22)	11572(1)	2193(1)	11528(2)	18(1)	1
C(23)	12787(1)	2299(1)	11669(2)	24(1)	1
C(24)	11282(2)	1946(1)	12567(2)	28(1)	1
C(25)	10911(2)	2556(1)	11562(2)	27(1)	1
C(26)	6939(1)	2612(1)	7809(1)	14(1)	1
C(27)	7674(2)	2869(1)	7112(2)	23(1)	1
C(28)	6950(2)	2751(1)	9079(2)	22(1)	1

C(29)	5770(1)	2638(1)	7266(2)	20(1)	1
C(30)	4438(1)	1232(1)	4172(1)	17(1)	1
C(31)	5131(2)	1156(1)	3117(2)	31(1)	1
C(32)	3364(2)	1012(1)	4015(2)	23(1)	1
C(33)	4134(2)	1648(1)	4186(2)	24(1)	1
C(34)	5539(1)	254(1)	7316(1)	15(1)	1
C(35)	6509(2)	-11(1)	7126(2)	21(1)	1
C(36)	4495(2)	58(1)	6813(2)	20(1)	1
C(37)	5416(1)	306(1)	8638(2)	19(1)	1
C(38)	8804(1)	1376(1)	4975(2)	19(1)	1
C(39)	9649(2)	1679(1)	5291(2)	24(1)	1
C(40)	10389(1)	789(1)	5337(1)	17(1)	1
C(41)	10552(2)	800(1)	4020(2)	24(1)	1
C(42)	8077(1)	621(1)	4917(2)	20(1)	1
C(43)	8386(2)	211(1)	4883(2)	27(1)	1
C(44)	10091(1)	988(1)	10862(2)	20(1)	1
C(45)	11005(2)	706(1)	10749(2)	33(1)	1
C(46)	8327(1)	465(1)	10333(1)	18(1)	1
C(47)	7976(2)	434(1)	11590(2)	30(1)	1
C(48)	7952(1)	1261(1)	10544(2)	18(1)	1
C(49)	6737(2)	1238(1)	10154(2)	24(1)	1

Table S51. Selected bond lengths [Å] and angles [°] for **15**.

Ir(1)-N(1)	2.0619(13)	N(1)-Ir(1)-O(2)	89.86(5)
Ir(1)-O(2)	2.0648(11)	N(1)-Ir(1)-O(1)	88.67(5)
Ir(1)-O(1)	2.0661(11)	O(2)-Ir(1)-O(1)	178.36(5)
Ir(1)-C(50)	2.148(7)	N(1)-Ir(1)-C(50)	177.12(15)
Ir(1)-P(1)	2.3711(4)	O(2)-Ir(1)-C(50)	89.65(17)
Ir(1)-P(2)	2.3722(4)	O(1)-Ir(1)-C(50)	91.86(17)
Ir(1)-I(2)	2.6625(3)	N(1)-Ir(1)-P(1)	93.81(4)
		O(2)-Ir(1)-P(1)	95.64(3)
		O(1)-Ir(1)-P(1)	83.74(3)
		C(50)-Ir(1)-P(1)	89.06(15)
		N(1)-Ir(1)-P(2)	91.30(4)
		O(2)-Ir(1)-P(2)	82.36(3)
		O(1)-Ir(1)-P(2)	98.40(3)
		C(50)-Ir(1)-P(2)	85.82(15)
		P(1)-Ir(1)-P(2)	174.510(14)
		N(1)-Ir(1)-I(2)	178.40(4)
		O(2)-Ir(1)-I(2)	91.65(3)
		O(1)-Ir(1)-I(2)	89.83(3)
		C(50)-Ir(1)-I(2)	3.05(16)
		P(1)-Ir(1)-I(2)	86.571(11)
		P(2)-Ir(1)-I(2)	88.374(11)

Table S52. Bond lengths [Å] and angles [°] for **15**.

Ir(1)-N(1)	2.0619(13)	C(8)-C(9)	1.395(2)
Ir(1)-O(2)	2.0648(11)	C(9)-C(10)	1.385(2)
Ir(1)-O(1)	2.0661(11)	C(9)-C(26)	1.531(2)
Ir(1)-C(50)	2.148(7)	C(10)-C(11)	1.403(2)
Ir(1)-P(1)	2.3711(4)	C(11)-C(12)	1.482(2)
Ir(1)-P(2)	2.3722(4)	C(12)-C(13)	1.410(2)
Ir(1)-I(2)	2.6625(3)	C(12)-C(17)	1.422(2)
P(1)-C(40)	1.8364(16)	C(13)-C(14)	1.377(2)
P(1)-C(38)	1.8432(18)	C(14)-C(15)	1.412(2)
P(1)-C(42)	1.8469(18)	C(14)-C(30)	1.532(2)
P(2)-C(44)	1.8322(18)	C(15)-C(16)	1.389(2)
P(2)-C(46)	1.8327(17)	C(16)-C(17)	1.437(2)
P(2)-C(48)	1.8409(16)	C(16)-C(34)	1.538(2)
O(1)-C(1)	1.3197(19)	C(18)-C(20)	1.535(3)
O(2)-C(17)	1.3218(19)	C(18)-C(21)	1.538(3)
N(1)-C(11)	1.3567(19)	C(18)-C(19)	1.538(3)
N(1)-C(7)	1.368(2)	C(22)-C(25)	1.530(3)
C(1)-C(6)	1.420(2)	C(22)-C(23)	1.534(2)
C(1)-C(2)	1.434(2)	C(22)-C(24)	1.539(3)
C(2)-C(3)	1.392(2)	C(26)-C(29)	1.529(2)
C(2)-C(18)	1.541(2)	C(26)-C(28)	1.535(2)
C(3)-C(4)	1.408(2)	C(26)-C(27)	1.542(2)
C(4)-C(5)	1.382(2)	C(30)-C(32)	1.533(2)
C(4)-C(22)	1.535(2)	C(30)-C(33)	1.534(3)
C(5)-C(6)	1.412(2)	C(30)-C(31)	1.542(2)
C(6)-C(7)	1.482(2)	C(34)-C(36)	1.539(2)
C(7)-C(8)	1.394(2)	C(34)-C(37)	1.543(2)

C(34)-C(35)	1.544(2)	C(40)-P(1)-C(38)	102.58(8)
C(38)-C(39)	1.527(3)	C(40)-P(1)-C(42)	104.13(8)
C(40)-C(41)	1.534(2)	C(38)-P(1)-C(42)	100.59(9)
C(42)-C(43)	1.514(3)	C(40)-P(1)-Ir(1)	112.10(6)
C(44)-C(45)	1.517(3)	C(38)-P(1)-Ir(1)	116.37(6)
C(46)-C(47)	1.531(2)	C(42)-P(1)-Ir(1)	119.00(6)
C(48)-C(49)	1.530(3)	C(44)-P(2)-C(46)	104.17(8)
		C(44)-P(2)-C(48)	99.26(8)
N(1)-Ir(1)-O(2)	89.86(5)	C(46)-P(2)-C(48)	103.83(8)
N(1)-Ir(1)-O(1)	88.67(5)	C(44)-P(2)-Ir(1)	120.85(6)
O(2)-Ir(1)-O(1)	178.36(5)	C(46)-P(2)-Ir(1)	111.27(6)
N(1)-Ir(1)-C(50)	177.12(15)	C(48)-P(2)-Ir(1)	115.43(6)
O(2)-Ir(1)-C(50)	89.65(17)	C(1)-O(1)-Ir(1)	118.27(9)
O(1)-Ir(1)-C(50)	91.86(17)	C(17)-O(2)-Ir(1)	118.62(9)
N(1)-Ir(1)-P(1)	93.81(4)	C(11)-N(1)-C(7)	119.56(13)
O(2)-Ir(1)-P(1)	95.64(3)	C(11)-N(1)-Ir(1)	120.35(10)
O(1)-Ir(1)-P(1)	83.74(3)	C(7)-N(1)-Ir(1)	120.08(10)
C(50)-Ir(1)-P(1)	89.06(15)	O(1)-C(1)-C(6)	122.73(13)
N(1)-Ir(1)-P(2)	91.30(4)	O(1)-C(1)-C(2)	119.70(13)
O(2)-Ir(1)-P(2)	82.36(3)	C(6)-C(1)-C(2)	117.55(14)
O(1)-Ir(1)-P(2)	98.40(3)	C(3)-C(2)-C(1)	118.20(13)
C(50)-Ir(1)-P(2)	85.82(15)	C(3)-C(2)-C(18)	120.95(14)
P(1)-Ir(1)-P(2)	174.510(14)	C(1)-C(2)-C(18)	120.72(14)
N(1)-Ir(1)-I(2)	178.40(4)	C(2)-C(3)-C(4)	124.04(15)
O(2)-Ir(1)-I(2)	91.65(3)	C(5)-C(4)-C(3)	116.24(15)
O(1)-Ir(1)-I(2)	89.83(3)	C(5)-C(4)-C(22)	121.90(14)
C(50)-Ir(1)-I(2)	3.05(16)	C(3)-C(4)-C(22)	121.79(14)
P(1)-Ir(1)-I(2)	86.571(11)	C(4)-C(5)-C(6)	122.43(14)
P(2)-Ir(1)-I(2)	88.374(11)	C(5)-C(6)-C(1)	119.77(14)

C(5)-C(6)-C(7)	117.20(13)	C(21)-C(18)-C(19)	106.59(16)
C(1)-C(6)-C(7)	122.80(14)	C(20)-C(18)-C(2)	113.17(15)
N(1)-C(7)-C(8)	120.28(13)	C(21)-C(18)-C(2)	112.57(15)
N(1)-C(7)-C(6)	121.96(13)	C(19)-C(18)-C(2)	107.41(14)
C(8)-C(7)-C(6)	117.76(13)	C(25)-C(22)-C(23)	107.32(15)
C(7)-C(8)-C(9)	121.34(14)	C(25)-C(22)-C(4)	111.44(15)
C(10)-C(9)-C(8)	116.76(14)	C(23)-C(22)-C(4)	111.91(13)
C(10)-C(9)-C(26)	123.51(13)	C(25)-C(22)-C(24)	108.50(16)
C(8)-C(9)-C(26)	119.73(14)	C(23)-C(22)-C(24)	109.19(16)
C(9)-C(10)-C(11)	121.20(14)	C(4)-C(22)-C(24)	108.41(15)
N(1)-C(11)-C(10)	120.53(14)	C(29)-C(26)-C(9)	112.45(13)
N(1)-C(11)-C(12)	121.90(13)	C(29)-C(26)-C(28)	108.72(13)
C(10)-C(11)-C(12)	117.56(13)	C(9)-C(26)-C(28)	109.06(13)
C(13)-C(12)-C(17)	119.25(14)	C(29)-C(26)-C(27)	108.42(14)
C(13)-C(12)-C(11)	116.47(13)	C(9)-C(26)-C(27)	109.04(12)
C(17)-C(12)-C(11)	124.11(14)	C(28)-C(26)-C(27)	109.10(15)
C(14)-C(13)-C(12)	123.10(14)	C(14)-C(30)-C(32)	111.88(14)
C(13)-C(14)-C(15)	116.08(14)	C(14)-C(30)-C(33)	111.66(14)
C(13)-C(14)-C(30)	120.63(14)	C(32)-C(30)-C(33)	106.96(14)
C(15)-C(14)-C(30)	123.24(14)	C(14)-C(30)-C(31)	108.30(14)
C(16)-C(15)-C(14)	123.90(14)	C(32)-C(30)-C(31)	109.14(16)
C(15)-C(16)-C(17)	118.23(14)	C(33)-C(30)-C(31)	108.85(16)
C(15)-C(16)-C(34)	121.36(14)	C(16)-C(34)-C(36)	112.13(14)
C(17)-C(16)-C(34)	120.39(14)	C(16)-C(34)-C(37)	109.55(13)
O(2)-C(17)-C(12)	122.72(14)	C(36)-C(34)-C(37)	107.12(13)
O(2)-C(17)-C(16)	119.49(14)	C(16)-C(34)-C(35)	111.13(12)
C(12)-C(17)-C(16)	117.79(14)	C(36)-C(34)-C(35)	107.26(14)
C(20)-C(18)-C(21)	107.25(16)	C(37)-C(34)-C(35)	109.53(14)
C(20)-C(18)-C(19)	109.65(16)	C(39)-C(38)-P(1)	114.44(13)

C(41)-C(40)-P(1)	115.62(12)
C(43)-C(42)-P(1)	116.35(14)
C(45)-C(44)-P(2)	116.28(14)
C(47)-C(46)-P(2)	116.69(14)
C(49)-C(48)-P(2)	116.67(12)

Table S53. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **15**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	99(1)	118(1)	86(1)	-5(1)	-4(1)	18(1)
I(2)	190(1)	126(1)	150(1)	12(1)	10(1)	50(1)
C(50)	220(20)	90(20)	160(20)	-74(18)	-10(18)	83(19)
P(1)	120(1)	185(2)	102(2)	-22(1)	2(1)	-6(1)
P(2)	144(2)	169(2)	90(2)	1(1)	2(1)	11(1)
O(1)	112(4)	168(5)	150(5)	-43(4)	6(4)	1(4)
O(2)	120(4)	144(5)	127(5)	21(4)	-18(4)	5(4)
N(1)	99(5)	130(5)	106(5)	-5(4)	-3(4)	7(4)
C(1)	107(5)	158(6)	115(6)	-3(5)	-2(5)	18(5)
C(2)	109(5)	182(7)	164(7)	-26(5)	-7(5)	30(5)
C(3)	109(6)	223(8)	172(7)	-39(6)	-31(5)	7(5)
C(4)	115(5)	163(7)	153(6)	-23(5)	-24(5)	4(5)
C(5)	113(5)	149(6)	148(6)	-19(5)	-14(5)	11(5)
C(6)	95(5)	139(6)	123(6)	-7(5)	-18(4)	14(4)
C(7)	103(5)	124(6)	121(6)	-7(4)	-4(4)	10(4)
C(8)	112(5)	113(6)	163(6)	-5(5)	-12(5)	2(5)
C(9)	119(5)	119(6)	133(6)	1(5)	-8(5)	18(5)
C(10)	111(5)	123(6)	156(6)	3(5)	-22(5)	19(5)
C(11)	108(5)	115(6)	117(6)	-3(4)	-14(4)	3(4)
C(12)	111(5)	118(6)	120(6)	-2(4)	-9(5)	0(4)
C(13)	123(5)	128(6)	135(6)	8(5)	-14(5)	0(5)
C(14)	127(5)	145(6)	126(6)	3(5)	-15(5)	-5(5)
C(15)	128(6)	135(6)	152(6)	1(5)	7(5)	-22(5)
C(16)	139(6)	117(6)	129(6)	-5(5)	17(5)	-13(5)

C(17)	122(5)	128(6)	106(6)	-1(4)	12(5)	0(5)
C(18)	103(6)	281(9)	225(8)	-76(6)	4(5)	44(6)
C(19)	181(7)	343(10)	238(8)	-49(7)	59(6)	7(7)
C(20)	179(7)	290(10)	327(10)	-41(7)	-7(7)	88(7)
C(21)	105(6)	493(13)	375(11)	-171(10)	-14(7)	46(7)
C(22)	140(6)	211(8)	168(7)	-50(6)	-33(5)	-8(5)
C(23)	162(7)	290(9)	266(9)	-95(7)	-35(6)	-29(6)
C(24)	294(9)	372(11)	173(8)	-9(7)	-20(7)	-61(8)
C(25)	233(8)	253(9)	304(10)	-133(7)	-71(7)	48(7)
C(26)	139(6)	117(6)	162(6)	-15(5)	-11(5)	27(5)
C(27)	233(8)	159(7)	303(9)	70(6)	35(7)	8(6)
C(28)	235(8)	212(8)	193(7)	-65(6)	-24(6)	67(6)
C(29)	177(6)	164(7)	246(8)	-27(6)	-49(6)	58(6)
C(30)	159(6)	206(7)	142(6)	19(5)	-40(5)	-20(6)
C(31)	301(9)	470(13)	150(8)	15(8)	10(7)	13(9)
C(32)	209(7)	224(8)	232(8)	16(6)	-90(6)	-56(6)
C(33)	212(7)	216(8)	264(9)	73(7)	-94(7)	-24(6)
C(34)	176(6)	133(6)	145(6)	17(5)	23(5)	-13(5)
C(35)	221(7)	142(7)	272(8)	7(6)	56(6)	11(6)
C(36)	211(7)	184(8)	216(8)	13(6)	12(6)	-73(6)
C(37)	189(7)	201(8)	175(7)	36(6)	34(6)	-14(6)
C(38)	184(7)	252(8)	145(7)	44(6)	0(6)	5(6)
C(39)	293(9)	221(8)	203(8)	53(6)	27(7)	-35(7)
C(40)	129(6)	245(8)	135(6)	-49(5)	12(5)	-16(5)
C(41)	188(7)	373(10)	154(7)	-67(7)	48(6)	-60(7)
C(42)	147(6)	309(9)	157(7)	-80(6)	10(5)	-32(6)
C(43)	237(8)	292(10)	288(9)	-119(7)	44(7)	-80(7)
C(44)	203(7)	254(8)	137(6)	20(6)	-41(5)	-10(6)
C(45)	190(8)	469(13)	321(11)	-35(9)	-88(7)	55(8)

C(46)	183(7)	209(8)	137(6)	42(5)	-1(5)	-12(6)
C(47)	342(10)	370(11)	178(8)	66(7)	66(7)	-74(8)
C(48)	204(7)	215(8)	137(6)	-39(5)	33(6)	19(6)
C(49)	192(7)	330(10)	193(8)	-64(7)	38(6)	44(7)

[(ONO^{tBu})Ir(PEt$_3$)$_2$Me]PF$_6$, 16

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The crystal is twinned and the twinning was explicitly incorporated into the integration of intensities and least squares refinement with the twin ratio of 62:38.

The asymmetric unit contains four discrete Ir-Me moieties and eight solvent sites; two at a center inversion and containing half of a benzene, two full occupancy benzene sites, two full occupancy hexafluorophosphate sites, and four sites with mixtures of benzene and hexafluorophosphate such that in total there are two additional benzene and hexafluorophosphate molecules (within error).

Restraints were placed on all anisotropic displacement parameters to approximate isotropic behavior. All partial occupancy benzenes were constrained to regular hexagons and in one site the temperature factors were fixed.

No restraints were placed on hexafluorophosphate.

Table S54. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **16**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ir(1)	837(1)	2532(1)	1980(1)	16(1)	1
P(1A)	1692(1)	2634(1)	1326(1)	17(1)	1
P(2A)	65(1)	2444(1)	2688(1)	21(1)	1
O(1A)	807(3)	3470(3)	1784(2)	21(2)	1
O(2A)	799(3)	1595(3)	2114(2)	18(1)	1
N(1A)	160(3)	2490(3)	1437(2)	7(2)	1
C(1A)	239(4)	3758(4)	1796(3)	15(2)	1

C(2A)	207(4)	4385(4)	1934(3)	16(2)	1
C(3A)	-385(4)	4648(4)	1991(3)	16(2)	1
C(4A)	-935(4)	4345(4)	1914(3)	20(2)	1
C(5A)	-879(4)	3769(4)	1744(3)	16(2)	1
C(6A)	-294(4)	3483(4)	1652(3)	17(2)	1
C(7A)	-292(4)	2932(4)	1388(3)	13(2)	1
C(8A)	-743(4)	2869(4)	1048(3)	13(2)	1
C(9A)	-792(4)	2355(4)	800(3)	14(2)	1
C(10A)	-313(4)	1900(4)	871(3)	17(2)	1
C(11A)	176(4)	1996(4)	1181(3)	11(2)	1
C(12A)	654(4)	1489(4)	1245(3)	13(2)	1
C(13A)	826(4)	1181(4)	830(3)	15(2)	1
C(14A)	1183(4)	647(4)	879(3)	16(2)	1
C(15A)	1323(4)	381(4)	1363(3)	19(2)	1
C(16A)	1188(4)	659(4)	1793(3)	19(2)	1
C(17A)	890(4)	1267(4)	1724(3)	18(2)	1
C(18A)	804(4)	4750(4)	2008(4)	27(2)	1
C(19A)	1180(5)	4861(5)	1478(4)	38(3)	1
C(20A)	1206(4)	4403(4)	2411(3)	28(2)	1
C(21A)	659(5)	5403(4)	2156(4)	34(3)	1
C(22A)	-1571(4)	4664(4)	2032(3)	21(2)	1
C(23A)	-1623(4)	4854(4)	2540(3)	32(3)	1
C(24A)	-1656(5)	5223(4)	1621(4)	41(3)	1
C(25A)	-2127(5)	4211(5)	2019(4)	52(3)	1
C(26A)	-1358(4)	2265(4)	494(3)	10(2)	1
C(27A)	-1419(4)	2843(4)	97(3)	28(2)	1
C(28A)	-1946(4)	2220(4)	887(3)	29(2)	1
C(29A)	-1306(4)	1665(4)	245(3)	24(2)	1
C(30A)	1393(4)	338(4)	397(3)	20(2)	1

C(31A)	823(4)	232(4)	104(3)	27(2)	1
C(32A)	1711(5)	-285(4)	524(4)	42(3)	1
C(33A)	1839(4)	797(4)	57(3)	29(2)	1
C(34A)	1274(4)	316(4)	2336(3)	26(2)	1
C(35A)	649(4)	193(4)	2629(3)	32(3)	1
C(36A)	1618(4)	-339(4)	2298(3)	33(3)	1
C(37A)	1707(4)	693(4)	2621(3)	28(2)	1
C(38A)	2230(4)	1973(4)	1282(3)	19(2)	1
C(39A)	2635(4)	1810(4)	1731(3)	31(2)	1
C(40A)	1455(4)	2834(4)	678(3)	18(2)	1
C(41A)	1156(4)	3459(4)	546(3)	20(2)	1
C(42A)	2215(4)	3287(4)	1401(3)	18(2)	1
C(43A)	2744(4)	3427(4)	980(3)	20(2)	1
C(44A)	322(5)	1852(5)	3191(4)	31(3)	1
C(45A)	-172(4)	1567(4)	3602(3)	34(3)	1
C(46A)	-740(4)	2220(4)	2584(3)	21(2)	1
C(47A)	-798(4)	1619(4)	2362(3)	20(2)	1
C(48A)	-48(4)	3150(4)	2985(3)	25(2)	1
C(49A)	-530(5)	3158(5)	3418(4)	56(3)	1
C(50A)	1480(4)	2603(4)	2530(3)	24(2)	1
Ir(2)	4109(1)	2647(1)	8542(1)	14(1)	1
P(1B)	3264(1)	2739(1)	9177(1)	15(1)	1
P(2B)	4867(1)	2570(1)	7840(1)	16(1)	1
O(1B)	4162(3)	3574(2)	8545(2)	15(1)	1
O(2B)	4134(3)	1712(2)	8595(2)	15(1)	1
N(1B)	4794(3)	2551(3)	9085(2)	13(2)	1
C(1B)	4718(4)	3871(4)	8466(3)	16(2)	1
C(2B)	4758(4)	4489(4)	8195(3)	12(2)	1

C(3B)	5358(4)	4738(4)	8084(3)	16(2)	1
C(4B)	5910(4)	4426(4)	8218(3)	15(2)	1
C(5B)	5864(4)	3862(4)	8505(3)	17(2)	1
C(6B)	5264(4)	3557(4)	8656(3)	12(2)	1
C(7B)	5249(4)	3004(4)	9059(3)	16(2)	1
C(8B)	5703(4)	2941(4)	9408(3)	15(2)	1
C(9B)	5758(4)	2392(4)	9753(3)	13(2)	1
C(10B)	5300(4)	1964(4)	9768(3)	12(2)	1
C(11B)	4806(4)	2030(4)	9444(3)	17(2)	1
C(12B)	4327(4)	1538(4)	9478(3)	13(2)	1
C(13B)	4215(4)	1161(4)	9960(3)	16(2)	1
C(14B)	3901(4)	604(4)	10018(3)	13(2)	1
C(15B)	3695(4)	403(4)	9587(3)	15(2)	1
C(16B)	3775(4)	748(4)	9100(3)	18(2)	1
C(17B)	4075(4)	1353(4)	9056(3)	14(2)	1
C(18B)	4184(4)	4866(4)	8062(3)	19(2)	1
C(19B)	3792(4)	4970(4)	8553(3)	23(2)	1
C(20B)	3759(4)	4520(4)	7723(3)	27(2)	1
C(21B)	4332(4)	5515(4)	7749(3)	28(2)	1
C(22B)	6553(5)	4737(4)	8079(4)	29(2)	1
C(23B)	6597(5)	4975(5)	7489(4)	38(3)	1
C(24B)	6597(5)	5336(4)	8337(4)	39(3)	1
C(25B)	7110(5)	4295(5)	8208(4)	43(3)	1
C(26B)	6317(4)	2323(4)	10080(3)	19(2)	1
C(27B)	6392(4)	2892(4)	10348(3)	28(2)	1
C(28B)	6898(4)	2232(4)	9717(3)	26(2)	1
C(29B)	6246(4)	1741(4)	10493(3)	20(2)	1
C(30B)	3849(4)	196(4)	10545(3)	17(2)	1
C(31B)	4498(4)	64(4)	10739(3)	23(2)	1

C(32B)	3531(4)	-441(4)	10529(3)	28(2)	1
C(33B)	3450(4)	559(4)	10911(3)	26(2)	1
C(34B)	3577(4)	467(4)	8625(3)	20(2)	1
C(35B)	4180(4)	324(4)	8324(3)	27(2)	1
C(36B)	3203(4)	-147(4)	8759(3)	28(2)	1
C(37B)	3149(4)	909(4)	8305(3)	31(2)	1
C(38B)	2702(4)	2096(4)	9318(3)	22(2)	1
C(39B)	2247(4)	2073(4)	8888(3)	31(2)	1
C(40B)	2780(4)	3438(4)	9004(3)	21(2)	1
C(41B)	2257(4)	3565(4)	9407(3)	29(2)	1
C(42B)	3491(4)	2842(4)	9798(3)	19(2)	1
C(43B)	3847(4)	3446(4)	9834(3)	26(2)	1
C(44B)	4624(4)	1984(4)	7454(3)	27(2)	1
C(45B)	4973(5)	1961(5)	6952(4)	41(3)	1
C(46B)	5661(4)	2317(4)	7994(3)	22(2)	1
C(47B)	5686(5)	1659(4)	8317(4)	33(3)	1
C(48B)	4968(4)	3290(4)	7376(3)	27(2)	1
C(49B)	5626(4)	3397(4)	7107(4)	34(3)	1
C(50B)	3453(4)	2778(4)	7975(3)	22(2)	1
Ir(3)	4516(1)	2554(1)	4023(1)	20(1)	1
P(1C)	5175(1)	2414(1)	4728(1)	25(1)	1
P(2C)	3738(1)	2670(1)	3414(1)	19(1)	1
O(1C)	4649(3)	3465(3)	3786(2)	21(2)	1
O(2C)	4461(3)	1634(3)	4194(2)	23(2)	1
N(1C)	5258(3)	2394(3)	3475(2)	14(2)	1
C(1C)	5222(5)	3701(4)	3795(3)	22(2)	1
C(2C)	5306(5)	4306(4)	3939(4)	30(2)	1
C(3C)	5902(5)	4504(5)	4008(4)	37(3)	1

C(4C)	6442(6)	4130(5)	3921(4)	51(3)	1
C(5C)	6361(5)	3562(4)	3732(4)	34(3)	1
C(6C)	5780(4)	3356(4)	3656(3)	23(2)	1
C(7C)	5743(4)	2817(4)	3375(3)	15(2)	1
C(8C)	6190(4)	2733(4)	2992(3)	32(2)	1
C(9C)	6193(4)	2248(4)	2718(3)	25(2)	1
C(10C)	5713(4)	1817(4)	2854(3)	26(2)	1
C(11C)	5231(4)	1889(4)	3228(3)	18(2)	1
C(12C)	4723(4)	1430(4)	3330(3)	15(2)	1
C(13C)	4594(4)	1057(4)	2955(3)	20(2)	1
C(14C)	4209(4)	554(4)	3042(3)	18(2)	1
C(15C)	3943(4)	376(4)	3538(4)	32(3)	1
C(16C)	4035(4)	702(4)	3946(3)	21(2)	1
C(17C)	4416(4)	1268(4)	3826(3)	24(2)	1
C(18C)	4746(5)	4750(5)	3997(4)	36(3)	1
C(19C)	4254(5)	4452(4)	4428(4)	38(3)	1
C(20C)	4423(5)	4846(5)	3492(4)	37(3)	1
C(21C)	4944(5)	5401(5)	4110(4)	51(3)	1
C(22C)	7101(6)	4365(6)	4053(5)	79(4)	1
C(23C)	7155(12)	4201(11)	4591(6)	273(14)	1
C(24C)	7177(13)	5055(8)	3848(10)	350(19)	1
C(25C)	7661(5)	4022(5)	3803(4)	64(4)	1
C(26C)	6672(5)	2211(5)	2272(4)	47(3)	1
C(27C)	6615(5)	2829(5)	1874(4)	48(3)	1
C(28C)	7336(5)	2229(6)	2462(4)	61(4)	1
C(29C)	6572(5)	1668(5)	1994(4)	54(3)	1
C(30C)	4069(4)	163(4)	2622(4)	27(2)	1
C(31C)	3350(4)	154(4)	2572(4)	38(3)	1
C(32C)	4298(5)	-511(5)	2787(4)	53(3)	1

C(33C)	4391(5)	408(5)	2122(4)	44(3)	1
C(34C)	3778(4)	474(4)	4498(3)	25(2)	1
C(35C)	4325(4)	334(4)	4816(4)	36(3)	1
C(36C)	3415(5)	-147(4)	4491(4)	43(3)	1
C(37C)	3332(4)	957(4)	4707(3)	35(3)	1
C(38C)	4780(4)	1892(4)	5262(3)	21(2)	1
C(39C)	5196(5)	1483(5)	5633(4)	49(3)	1
C(40C)	5960(4)	2082(4)	4601(3)	26(2)	1
C(41C)	5972(5)	1446(4)	4420(3)	33(3)	1
C(42C)	5344(5)	3139(4)	4989(3)	31(3)	1
C(43C)	5681(5)	3040(5)	5482(4)	63(4)	1
C(44C)	3125(4)	2053(4)	3551(3)	29(2)	1
C(45C)	2931(4)	1771(4)	3101(4)	36(3)	1
C(46C)	4013(4)	2704(4)	2746(3)	22(2)	1
C(47C)	4458(5)	3287(4)	2559(4)	32(3)	1
C(48C)	3276(4)	3396(4)	3430(3)	28(2)	1
C(49C)	2746(5)	3460(4)	3056(4)	34(3)	1
C(50C)	3749(4)	2725(4)	4557(3)	21(2)	1
Ir(4)	10401(1)	2671(1)	6460(1)	25(1)	1
P(1D)	9688(1)	2567(1)	5812(1)	28(1)	1
P(2D)	11216(1)	2757(1)	7015(1)	25(1)	1
O(1D)	10298(3)	3580(3)	6504(2)	25(2)	1
O(2D)	10419(3)	1739(3)	6499(2)	28(2)	1
N(1D)	9681(3)	2514(3)	7057(2)	16(2)	1
C(1D)	9720(5)	3842(4)	6455(3)	27(2)	1
C(2D)	9660(5)	4472(4)	6197(3)	27(2)	1
C(3D)	9073(5)	4683(5)	6100(3)	31(2)	1
C(4D)	8532(5)	4333(4)	6251(3)	27(2)	1

C(5D)	8587(4)	3759(4)	6555(3)	24(2)	1
C(6D)	9193(4)	3513(4)	6670(3)	22(2)	1
C(7D)	9208(4)	2948(4)	7074(3)	21(2)	1
C(8D)	8761(4)	2896(4)	7487(3)	19(2)	1
C(9D)	8772(4)	2391(4)	7870(3)	28(2)	1
C(10D)	9234(4)	1942(4)	7831(3)	19(2)	1
C(11D)	9706(4)	2017(4)	7426(3)	17(2)	1
C(12D)	10185(4)	1534(4)	7396(3)	17(2)	1
C(13D)	10338(4)	1165(4)	7858(3)	20(2)	1
C(14D)	10731(4)	650(4)	7867(3)	23(2)	1
C(15D)	10948(4)	472(4)	7415(3)	24(2)	1
C(16D)	10824(4)	805(4)	6948(3)	27(2)	1
C(17D)	10489(4)	1364(4)	6937(4)	25(2)	1
C(18D)	10251(5)	4890(5)	6040(4)	34(3)	1
C(19D)	10708(5)	4597(5)	5664(4)	47(3)	1
C(20D)	10570(5)	4964(4)	6518(3)	30(3)	1
C(21D)	10087(5)	5552(5)	5797(4)	47(3)	1
C(22D)	7895(5)	4603(5)	6105(4)	44(3)	1
C(23D)	7922(5)	4862(5)	5559(4)	56(3)	1
C(24D)	7736(4)	5141(4)	6398(3)	25(2)	1
C(25D)	7377(6)	4125(5)	6225(5)	71(4)	1
C(26D)	8278(5)	2344(5)	8312(4)	34(3)	1
C(27D)	7626(5)	2366(5)	8119(4)	57(3)	1
C(28D)	8317(5)	2952(5)	8579(4)	46(3)	1
C(29D)	8358(5)	1803(5)	8724(4)	45(3)	1
C(30D)	10919(4)	275(4)	8378(4)	24(2)	1
C(31D)	11284(5)	682(5)	8646(4)	59(4)	1
C(32D)	10355(6)	61(6)	8706(5)	83(4)	1
C(33D)	11368(6)	-258(6)	8310(5)	83(4)	1

C(34D)	11050(5)	540(5)	6438(4)	39(3)	1
C(35D)	10445(5)	399(5)	6180(4)	44(3)	1
C(36D)	11468(5)	999(5)	6086(4)	48(3)	1
C(37D)	11438(5)	-63(5)	6526(4)	53(3)	1
C(38D)	10022(5)	2039(5)	5391(4)	36(3)	1
C(39D)	9620(5)	1882(5)	4981(4)	56(3)	1
C(40D)	9529(5)	3286(4)	5397(4)	35(3)	1
C(41D)	8895(5)	3328(5)	5170(4)	51(3)	1
C(42D)	8912(5)	2224(4)	6046(4)	34(3)	1
C(43D)	8946(5)	1556(4)	6332(4)	43(3)	1
C(44D)	11806(5)	2129(5)	6973(4)	49(3)	1
C(45D)	12124(5)	1863(5)	7426(4)	61(4)	1
C(46D)	10968(4)	2776(4)	7673(3)	24(2)	1
C(47D)	10578(5)	3337(4)	7782(3)	32(3)	1
C(48D)	11668(5)	3485(4)	6840(4)	38(3)	1
C(49D)	12203(5)	3574(5)	7181(4)	45(3)	1
C(50D)	11093(4)	2824(4)	5863(4)	33(3)	1
C(1E)	10094(5)	4604(5)	-374(4)	40(3)	1
C(2E)	9873(5)	4384(5)	115(4)	40(3)	1
C(3E)	9791(4)	4760(5)	484(4)	34(3)	1
C(1F)	5227(5)	4755(5)	-419(4)	42(3)	1
C(2F)	5114(5)	4366(5)	18(4)	41(3)	1
C(3F)	4891(5)	4614(5)	440(4)	47(3)	1
C(1G)	2636(4)	5637(3)	9385(2)	86(5)	1
C(2G)	3126(3)	5428(4)	9683(3)	67(4)	1
C(3G)	2996(4)	5124(4)	10176(3)	57(3)	1

C(4G)	2377(4)	5027(3)	10370(2)	103(5)	1
C(5G)	1887(3)	5236(4)	10072(3)	50(3)	1
C(6G)	2017(4)	5540(3)	9579(3)	68(4)	1
C(1H)	3094(7)	672(9)	6241(6)	370(20)	1
C(2H)	3246(7)	59(9)	6169(5)	174(8)	1
C(3H)	3688(7)	-274(6)	6459(6)	171(9)	1
C(4H)	3978(5)	6(7)	6820(5)	158(8)	1
C(5H)	3826(7)	619(7)	6893(5)	131(7)	1
C(6H)	3384(8)	952(6)	6603(7)	670(50)	1
C(1I)	1365(10)	1052(7)	4306(7)	207(10)	1
C(2I)	1728(7)	632(10)	4058(5)	218(11)	1
C(3I)	1593(8)	-8(9)	4153(6)	154(8)	1
C(4I)	1096(10)	-227(7)	4497(8)	420(20)	1
C(5I)	733(8)	193(12)	4746(7)	301(15)	1
C(6I)	868(10)	832(11)	4650(7)	520(30)	1
P(1)	7049(5)	2052(4)	6679(3)	45(2)	0.406(6)
F(1A)	7177(7)	1476(6)	6470(5)	42(4)	0.406(6)
F(2A)	7385(8)	2456(8)	6201(6)	75(6)	0.406(6)
F(3A)	6942(7)	2687(7)	6995(5)	57(5)	0.406(6)
F(4A)	6695(7)	1689(7)	7187(6)	53(5)	0.406(6)
F(5A)	6432(8)	2176(8)	6469(6)	74(6)	0.406(6)
F(6A)	7701(8)	2064(8)	6927(7)	77(6)	0.406(6)
C(1J)	7400(7)	1518(7)	5882(5)	80	0.594(6)
C(2J)	7251(7)	2154(7)	5838(5)	80	0.594(6)
C(3J)	7092(8)	2430(6)	6271(7)	80	0.594(6)

C(4J)	7082(9)	2070(8)	6749(5)	80	0.594(6)
C(5J)	7231(8)	1435(8)	6793(5)	80	0.594(6)
C(6J)	7390(7)	1158(6)	6360(6)	80	0.594(6)
P(2)	4499(1)	2345(1)	1223(1)	30(1)	1
F(1B)	4199(3)	2031(3)	1755(2)	48(2)	1
F(2B)	4817(3)	2690(3)	683(2)	54(2)	1
F(3B)	3893(3)	2208(3)	951(2)	38(2)	1
F(4B)	4782(3)	1678(3)	1107(2)	43(2)	1
F(5B)	5124(3)	2466(3)	1500(3)	68(2)	1
F(6B)	4223(3)	3013(3)	1330(2)	52(2)	1
P(3)	429(1)	2462(1)	9347(1)	29(1)	1
F(1C)	168(3)	2750(3)	9846(2)	50(2)	1
F(2C)	689(3)	2158(3)	8852(2)	43(2)	1
F(3C)	-193(3)	2656(3)	9079(2)	60(2)	1
F(4C)	758(3)	3109(3)	9111(2)	49(2)	1
F(5C)	132(3)	1811(3)	9593(2)	62(2)	1
F(6C)	1049(2)	2291(3)	9633(2)	36(2)	1
P(4)	1295(2)	3049(2)	4205(2)	28(1)	0.562(5)
F(1D)	596(4)	2743(4)	4250(3)	16(2)	0.562(5)
F(2D)	1414(5)	2506(4)	4684(4)	38(3)	0.562(5)
F(3D)	1526(5)	2540(5)	3824(4)	47(3)	0.562(5)
F(4D)	1163(5)	3554(4)	3736(4)	42(3)	0.562(5)
F(5D)	1985(5)	3274(5)	4192(4)	49(3)	0.562(5)
F(6D)	1071(5)	3520(5)	4595(4)	44(3)	0.562(5)
C(1K)	1439(9)	2934(11)	4261(8)	80	0.438(5)

C(2K)	1528(9)	2291(10)	4388(8)	80	0.438(5)
C(3K)	1951(10)	2069(7)	4745(8)	80	0.438(5)
C(4K)	2284(8)	2490(10)	4975(7)	80	0.438(5)
C(5K)	2195(9)	3133(9)	4848(8)	80	0.438(5)
C(6K)	1772(10)	3355(8)	4491(8)	80	0.438(5)
P(5)	3633(3)	3119(3)	6168(3)	29(2)	0.479(6)
F(1E)	4324(5)	2866(5)	6216(4)	33(3)	0.479(6)
F(2E)	3791(6)	3663(6)	6521(5)	57(4)	0.479(6)
F(3E)	3803(7)	3639(6)	5677(5)	71(5)	0.479(6)
F(4E)	3440(6)	2599(6)	5855(5)	42(4)	0.479(6)
F(5E)	3434(6)	2658(6)	6682(5)	47(4)	0.479(6)
F(6E)	2919(6)	3373(5)	6161(5)	49(4)	0.479(6)
C(1L)	3474(9)	3139(10)	6024(8)	150(20)	0.521(6)
C(2L)	3547(8)	2497(11)	6169(7)	126(13)	0.521(6)
C(3L)	3185(9)	2072(7)	5968(7)	83(9)	0.521(6)
C(4L)	2748(7)	2289(7)	5621(6)	68(8)	0.521(6)
C(5L)	2674(7)	2932(8)	5476(5)	41(5)	0.521(6)
C(6L)	3037(9)	3357(6)	5677(7)	107(11)	0.521(6)
P(6)	7865(4)	1866(4)	4049(3)	56(3)	0.459(7)
F(2F)	7652(8)	1264(7)	4341(7)	90(6)	0.459(7)
F(1F)	7232(7)	1876(7)	3742(6)	83(6)	0.459(7)
F(5F)	7452(10)	2308(9)	4325(7)	104(7)	0.459(7)
F(3F)	8180(8)	1534(7)	3595(6)	91(6)	0.459(7)
F(4F)	8003(9)	2436(9)	3650(8)	125(8)	0.459(7)
F(6F)	8471(12)	2045(11)	4302(9)	159(10)	0.459(7)

C(1M)	8051(10)	1515(11)	4187(7)	104(11)	0.541(7)
C(2M)	7982(9)	1097(7)	4636(10)	107(10)	0.541(7)
C(3M)	7748(9)	1306(8)	5084(7)	116(11)	0.541(7)
C(4M)	7583(8)	1934(9)	5082(6)	97(10)	0.541(7)
C(5M)	7652(9)	2352(7)	4633(8)	60(7)	0.541(7)
C(6M)	7886(11)	2143(10)	4185(6)	220(30)	0.541(7)

Table S55. Selected bond lengths [Å] and angles [°] for **16.**

Ir(1)-O(2A)	1.994(5)	Ir(3)-O(2C)	1.967(6)
Ir(1)-O(1A)	2.011(5)	Ir(3)-O(1C)	1.987(6)
Ir(1)-C(50A)	2.101(8)	Ir(3)-N(1C)	2.131(6)
Ir(1)-N(1A)	2.129(7)	Ir(3)-C(50C)	2.153(8)
Ir(1)-P(2A)	2.400(2)	Ir(3)-P(2C)	2.390(2)
Ir(1)-P(1A)	2.418(2)	Ir(3)-P(1C)	2.410(3)
Ir(2)-O(2B)	1.993(5)	Ir(4)-O(1D)	1.982(6)
Ir(2)-O(1B)	1.997(5)	Ir(4)-O(2D)	1.989(6)
Ir(2)-N(1B)	2.118(7)	Ir(4)-C(50D)	2.081(8)
Ir(2)-C(50B)	2.119(8)	Ir(4)-N(1D)	2.122(7)
Ir(2)-P(2B)	2.403(2)	Ir(4)-P(2D)	2.388(3)
Ir(2)-P(1B)	2.408(2)	Ir(4)-P(1D)	2.414(3)
O(2A)-Ir(1)-O(1A)	173.5(2)	C(50A)-Ir(1)-P(1A)	89.8(2)
O(2A)-Ir(1)-C(50A)	94.2(3)	N(1A)-Ir(1)-P(1A)	91.96(18)
O(1A)-Ir(1)-C(50A)	92.3(3)	P(2A)-Ir(1)-P(1A)	174.24(8)
O(2A)-Ir(1)-N(1A)	87.4(2)		
O(1A)-Ir(1)-N(1A)	86.1(2)	O(2B)-Ir(2)-O(1B)	173.4(2)
C(50A)-Ir(1)-N(1A)	177.4(3)	O(2B)-Ir(2)-N(1B)	86.3(2)
O(2A)-Ir(1)-P(2A)	82.62(17)	O(1B)-Ir(2)-N(1B)	87.1(2)
O(1A)-Ir(1)-P(2A)	98.06(18)	O(2B)-Ir(2)-C(50B)	95.6(3)
C(50A)-Ir(1)-P(2A)	84.4(2)	O(1B)-Ir(2)-C(50B)	91.0(3)
N(1A)-Ir(1)-P(2A)	93.78(18)	N(1B)-Ir(2)-C(50B)	177.1(3)
O(2A)-Ir(1)-P(1A)	98.16(17)	O(2B)-Ir(2)-P(2B)	82.09(17)
O(1A)-Ir(1)-P(1A)	81.81(18)	O(1B)-Ir(2)-P(2B)	98.13(17)

N(1B)-Ir(2)-P(2B)	93.62(19)	N(1C)-Ir(3)-P(1C)	94.24(19)
C(50B)-Ir(2)-P(2B)	84.5(2)	C(50C)-Ir(3)-P(1C)	87.5(2)
O(2B)-Ir(2)-P(1B)	98.47(17)	P(2C)-Ir(3)-P(1C)	171.73(9)
O(1B)-Ir(2)-P(1B)	82.05(17)		
N(1B)-Ir(2)-P(1B)	92.72(19)	O(1D)-Ir(4)-O(2D)	172.1(2)
C(50B)-Ir(2)-P(1B)	89.2(2)	O(1D)-Ir(4)-C(50D)	93.3(3)
P(2B)-Ir(2)-P(1B)	173.65(8)	O(2D)-Ir(4)-C(50D)	94.6(3)
O(2C)-Ir(3)-O(1C)	173.2(2)	O(1D)-Ir(4)-N(1D)	86.8(3)
O(2C)-Ir(3)-N(1C)	86.6(3)	O(2D)-Ir(4)-N(1D)	85.3(3)
O(1C)-Ir(3)-N(1C)	86.6(2)	C(50D)-Ir(4)-N(1D)	178.8(3)
O(2C)-Ir(3)-C(50C)	94.1(3)	O(1D)-Ir(4)-P(2D)	82.83(19)
O(1C)-Ir(3)-C(50C)	92.7(3)	O(2D)-Ir(4)-P(2D)	97.0(2)
N(1C)-Ir(3)-C(50C)	178.3(3)	C(50D)-Ir(4)-P(2D)	86.8(3)
O(2C)-Ir(3)-P(2C)	97.05(19)	N(1D)-Ir(4)-P(2D)	94.3(2)
O(1C)-Ir(3)-P(2C)	83.01(18)	O(1D)-Ir(4)-P(1D)	99.65(19)
N(1C)-Ir(3)-P(2C)	93.64(19)	O(2D)-Ir(4)-P(1D)	81.6(2)
C(50C)-Ir(3)-P(2C)	84.7(2)	C(50D)-Ir(4)-P(1D)	85.7(3)
O(2C)-Ir(3)-P(1C)	80.95(19)	N(1D)-Ir(4)-P(1D)	93.1(2)
O(1C)-Ir(3)-P(1C)	99.94(18)	P(2D)-Ir(4)-P(1D)	172.30(9)

Symmetry transformations used to generate equivalent atoms:

Table S56. Bond lengths [Å] and angles [°] for **16**.

Ir(1)-O(2A)	1.994(5)	C(9A)-C(10A)	1.412(10)
Ir(1)-O(1A)	2.011(5)	C(9A)-C(26A)	1.532(11)
Ir(1)-C(50A)	2.101(8)	C(10A)-C(11A)	1.410(11)
Ir(1)-N(1A)	2.129(7)	C(11A)-C(12A)	1.486(10)
Ir(1)-P(2A)	2.400(2)	C(12A)-C(13A)	1.392(10)
Ir(1)-P(1A)	2.418(2)	C(12A)-C(17A)	1.422(11)
P(1A)-C(40A)	1.826(8)	C(13A)-C(14A)	1.369(10)
P(1A)-C(38A)	1.830(8)	C(14A)-C(15A)	1.386(11)
P(1A)-C(42A)	1.842(8)	C(14A)-C(30A)	1.562(11)
P(2A)-C(48A)	1.812(8)	C(15A)-C(16A)	1.377(11)
P(2A)-C(44A)	1.822(9)	C(16A)-C(17A)	1.442(11)
P(2A)-C(46A)	1.840(9)	C(16A)-C(34A)	1.548(11)
O(1A)-C(1A)	1.355(9)	C(18A)-C(20A)	1.529(12)
O(2A)-C(17A)	1.336(9)	C(18A)-C(21A)	1.535(11)
N(1A)-C(11A)	1.339(10)	C(18A)-C(19A)	1.559(12)
N(1A)-C(7A)	1.347(9)	C(22A)-C(23A)	1.464(11)
C(1A)-C(6A)	1.388(11)	C(22A)-C(24A)	1.524(11)
C(1A)-C(2A)	1.446(11)	C(22A)-C(25A)	1.546(10)
C(2A)-C(3A)	1.386(11)	C(26A)-C(27A)	1.523(10)
C(2A)-C(18A)	1.542(12)	C(26A)-C(29A)	1.532(11)
C(3A)-C(4A)	1.392(11)	C(26A)-C(28A)	1.569(11)
C(4A)-C(5A)	1.378(11)	C(30A)-C(32A)	1.501(11)
C(4A)-C(22A)	1.546(11)	C(30A)-C(31A)	1.528(11)
C(5A)-C(6A)	1.407(11)	C(30A)-C(33A)	1.529(11)
C(6A)-C(7A)	1.459(11)	C(34A)-C(35A)	1.503(12)
C(7A)-C(8A)	1.388(11)	C(34A)-C(37A)	1.542(12)
C(8A)-C(9A)	1.373(11)	C(34A)-C(36A)	1.594(11)

C(38A)-C(39A)	1.525(10)	C(5B)-C(6B)	1.447(11)
C(40A)-C(41A)	1.488(10)	C(6B)-C(7B)	1.483(11)
C(42A)-C(43A)	1.531(10)	C(7B)-C(8B)	1.384(11)
C(44A)-C(45A)	1.528(11)	C(8B)-C(9B)	1.397(10)
C(46A)-C(47A)	1.503(11)	C(9B)-C(10B)	1.342(11)
C(48A)-C(49A)	1.490(11)	C(9B)-C(26B)	1.521(11)
Ir(2)-O(2B)	1.993(5)	C(10B)-C(11B)	1.403(11)
Ir(2)-O(1B)	1.997(5)	C(11B)-C(12B)	1.467(11)
Ir(2)-N(1B)	2.118(7)	C(12B)-C(17B)	1.388(11)
Ir(2)-C(50B)	2.119(8)	C(12B)-C(13B)	1.422(10)
Ir(2)-P(2B)	2.403(2)	C(13B)-C(14B)	1.362(11)
Ir(2)-P(1B)	2.408(2)	C(14B)-C(15B)	1.384(11)
P(1B)-C(42B)	1.799(8)	C(14B)-C(30B)	1.544(11)
P(1B)-C(38B)	1.818(9)	C(15B)-C(16B)	1.398(10)
P(1B)-C(40B)	1.838(8)	C(16B)-C(17B)	1.442(11)
P(2B)-C(46B)	1.832(9)	C(16B)-C(34B)	1.563(11)
P(2B)-C(44B)	1.835(9)	C(18B)-C(19B)	1.542(11)
P(2B)-C(48B)	1.842(9)	C(18B)-C(21B)	1.544(11)
O(1B)-C(1B)	1.342(9)	C(18B)-C(20B)	1.586(12)
O(2B)-C(17B)	1.352(9)	C(22B)-C(25B)	1.541(12)
N(1B)-C(11B)	1.366(10)	C(22B)-C(24B)	1.549(12)
N(1B)-C(7B)	1.371(10)	C(22B)-C(23B)	1.577(12)
C(1B)-C(2B)	1.418(11)	C(26B)-C(27B)	1.515(11)
C(1B)-C(6B)	1.428(11)	C(26B)-C(29B)	1.543(11)
C(2B)-C(3B)	1.388(11)	C(26B)-C(28B)	1.544(11)
C(2B)-C(18B)	1.498(11)	C(30B)-C(31B)	1.522(11)
C(3B)-C(4B)	1.395(11)	C(30B)-C(33B)	1.537(11)
C(4B)-C(5B)	1.339(10)	C(30B)-C(32B)	1.540(11)
C(4B)-C(22B)	1.529(12)	C(34B)-C(35B)	1.517(11)

C(34B)-C(37B)	1.525(11)	C(4C)-C(5C)	1.402(13)
C(34B)-C(36B)	1.532(11)	C(4C)-C(22C)	1.576(15)
C(38B)-C(39B)	1.559(11)	C(5C)-C(6C)	1.359(12)
C(40B)-C(41B)	1.540(11)	C(6C)-C(7C)	1.471(11)
C(42B)-C(43B)	1.529(11)	C(7C)-C(8C)	1.374(11)
C(44B)-C(45B)	1.489(11)	C(8C)-C(9C)	1.355(12)
C(46B)-C(47B)	1.550(11)	C(9C)-C(10C)	1.380(12)
C(48B)-C(49B)	1.534(11)	C(9C)-C(26C)	1.522(13)
Ir(3)-O(2C)	1.967(6)	C(10C)-C(11C)	1.402(11)
Ir(3)-O(1C)	1.987(6)	C(11C)-C(12C)	1.458(11)
Ir(3)-N(1C)	2.131(6)	C(12C)-C(13C)	1.409(11)
Ir(3)-C(50C)	2.153(8)	C(12C)-C(17C)	1.428(11)
Ir(3)-P(2C)	2.390(2)	C(13C)-C(14C)	1.346(11)
Ir(3)-P(1C)	2.410(3)	C(14C)-C(15C)	1.402(12)
P(1C)-C(38C)	1.838(8)	C(14C)-C(30C)	1.537(12)
P(1C)-C(40C)	1.841(9)	C(15C)-C(16C)	1.401(12)
P(1C)-C(42C)	1.843(9)	C(16C)-C(17C)	1.455(12)
P(2C)-C(46C)	1.823(8)	C(16C)-C(34C)	1.544(11)
P(2C)-C(48C)	1.842(9)	C(18C)-C(21C)	1.541(13)
P(2C)-C(44C)	1.852(9)	C(18C)-C(20C)	1.543(12)
O(1C)-C(1C)	1.330(10)	C(18C)-C(19C)	1.568(13)
O(2C)-C(17C)	1.349(10)	C(22C)-C(23C)	1.439(13)
N(1C)-C(11C)	1.350(10)	C(22C)-C(24C)	1.510(13)
N(1C)-C(7C)	1.370(10)	C(22C)-C(25C)	1.556(11)
C(1C)-C(2C)	1.422(12)	C(26C)-C(29C)	1.492(13)
C(1C)-C(6C)	1.449(12)	C(26C)-C(28C)	1.540(14)
C(2C)-C(3C)	1.378(13)	C(26C)-C(27C)	1.588(13)
C(2C)-C(18C)	1.535(13)	C(30C)-C(33C)	1.481(12)
C(3C)-C(4C)	1.423(13)	C(30C)-C(32C)	1.540(12)

C(30C)-C(31C)	1.551(12)	C(2D)-C(18D)	1.551(13)
C(34C)-C(35C)	1.494(12)	C(3D)-C(4D)	1.385(12)
C(34C)-C(37C)	1.536(11)	C(4D)-C(5D)	1.385(11)
C(34C)-C(36C)	1.551(12)	C(4D)-C(22D)	1.527(13)
C(38C)-C(39C)	1.549(11)	C(5D)-C(6D)	1.430(11)
C(40C)-C(41C)	1.513(12)	C(6D)-C(7D)	1.505(11)
C(42C)-C(43C)	1.528(13)	C(7D)-C(8D)	1.394(11)
C(44C)-C(45C)	1.502(12)	C(8D)-C(9D)	1.381(11)
C(46C)-C(47C)	1.579(11)	C(9D)-C(10D)	1.380(11)
C(48C)-C(49C)	1.551(12)	C(9D)-C(26D)	1.515(12)
Ir(4)-O(1D)	1.982(6)	C(10D)-C(11D)	1.414(11)
Ir(4)-O(2D)	1.989(6)	C(11D)-C(12D)	1.457(11)
Ir(4)-C(50D)	2.081(8)	C(12D)-C(13D)	1.422(11)
Ir(4)-N(1D)	2.122(7)	C(12D)-C(17D)	1.434(11)
Ir(4)-P(2D)	2.388(3)	C(13D)-C(14D)	1.380(11)
Ir(4)-P(1D)	2.414(3)	C(14D)-C(15D)	1.362(11)
P(1D)-C(38D)	1.812(9)	C(14D)-C(30D)	1.559(12)
P(1D)-C(40D)	1.812(9)	C(15D)-C(16D)	1.385(11)
P(1D)-C(42D)	1.847(10)	C(16D)-C(17D)	1.391(11)
P(2D)-C(46D)	1.798(8)	C(16D)-C(34D)	1.587(12)
P(2D)-C(48D)	1.829(10)	C(18D)-C(20D)	1.515(12)
P(2D)-C(44D)	1.847(10)	C(18D)-C(21D)	1.525(12)
O(1D)-C(1D)	1.358(10)	C(18D)-C(19D)	1.542(13)
O(2D)-C(17D)	1.335(10)	C(22D)-C(23D)	1.477(13)
N(1D)-C(11D)	1.348(10)	C(22D)-C(25D)	1.505(14)
N(1D)-C(7D)	1.370(10)	C(22D)-C(24D)	1.505(12)
C(1D)-C(6D)	1.378(12)	C(26D)-C(29D)	1.500(12)
C(1D)-C(2D)	1.438(12)	C(26D)-C(27D)	1.515(14)
C(2D)-C(3D)	1.358(12)	C(26D)-C(28D)	1.578(13)

C(30D)-C(31D)	1.466(13)	C(3H)-C(4H)	1.3900
C(30D)-C(32D)	1.472(13)	C(4H)-C(5H)	1.3900
C(30D)-C(33D)	1.506(13)	C(5H)-C(6H)	1.3900
C(34D)-C(36D)	1.510(13)	C(1I)-C(2I)	1.3900
C(34D)-C(37D)	1.531(12)	C(1I)-C(6I)	1.3900
C(34D)-C(35D)	1.558(14)	C(2I)-C(3I)	1.3900
C(38D)-C(39D)	1.511(13)	C(3I)-C(4I)	1.3900
C(40D)-C(41D)	1.518(13)	C(4I)-C(5I)	1.3900
C(42D)-C(43D)	1.531(12)	C(5I)-C(6I)	1.3900
C(44D)-C(45D)	1.469(13)	P(1)-F(1A)	1.445(15)
C(46D)-C(47D)	1.509(11)	P(1)-F(5A)	1.474(19)
C(48D)-C(49D)	1.540(13)	P(1)-F(2A)	1.565(18)
C(1E)-C(2E)	1.373(13)	P(1)-F(6A)	1.58(2)
C(1E)-C(3E)#1	1.377(13)	P(1)-F(4A)	1.604(17)
C(2E)-C(3E)	1.358(13)	P(1)-F(3A)	1.705(17)
C(3E)-C(1E)#1	1.377(13)	C(1J)-C(2J)	1.3900
C(1F)-C(2F)	1.341(13)	C(1J)-C(6J)	1.3900
C(1F)-C(3F)#2	1.370(13)	C(2J)-C(3J)	1.3900
C(2F)-C(3F)	1.363(13)	C(3J)-C(4J)	1.3900
C(3F)-C(1F)#2	1.370(13)	C(4J)-C(5J)	1.3900
C(1G)-C(2G)	1.3900	C(5J)-C(6J)	1.3900
C(1G)-C(6G)	1.3900	P(2)-F(1B)	1.575(6)
C(2G)-C(3G)	1.3900	P(2)-F(3B)	1.577(6)
C(3G)-C(4G)	1.3900	P(2)-F(6B)	1.600(6)
C(4G)-C(5G)	1.3900	P(2)-F(4B)	1.610(6)
C(5G)-C(6G)	1.3900	P(2)-F(5B)	1.611(6)
C(1H)-C(2H)	1.3900	P(2)-F(2B)	1.625(6)
C(1H)-C(6H)	1.3900	P(3)-F(5C)	1.576(6)
C(2H)-C(3H)	1.3900	P(3)-F(3C)	1.578(6)

P(3)-F(6C)	1.588(5)	P(6)-F(5F)	1.52(2)
P(3)-F(4C)	1.590(6)	P(6)-F(4F)	1.52(2)
P(3)-F(1C)	1.605(6)	P(6)-F(6F)	1.58(3)
P(3)-F(2C)	1.613(6)	P(6)-F(3F)	1.593(18)
P(4)-F(5D)	1.551(11)	P(6)-F(1F)	1.627(18)
P(4)-F(4D)	1.575(10)	C(1M)-C(2M)	1.3900
P(4)-F(6D)	1.597(11)	C(1M)-C(6M)	1.3900
P(4)-F(1D)	1.624(9)	C(2M)-C(3M)	1.3900
P(4)-F(2D)	1.633(10)	C(3M)-C(4M)	1.3900
P(4)-F(3D)	1.645(11)	C(4M)-C(5M)	1.3900
C(1K)-C(2K)	1.3900	C(5M)-C(6M)	1.3900
C(1K)-C(6K)	1.3900		
C(2K)-C(3K)	1.3900	O(2A)-Ir(1)-O(1A)	173.5(2)
C(3K)-C(4K)	1.3900	O(2A)-Ir(1)-C(50A)	94.2(3)
C(4K)-C(5K)	1.3900	O(1A)-Ir(1)-C(50A)	92.3(3)
C(5K)-C(6K)	1.3900	O(2A)-Ir(1)-N(1A)	87.4(2)
P(5)-F(4E)	1.560(13)	O(1A)-Ir(1)-N(1A)	86.1(2)
P(5)-F(1E)	1.574(12)	C(50A)-Ir(1)-N(1A)	177.4(3)
P(5)-F(5E)	1.604(13)	O(2A)-Ir(1)-P(2A)	82.62(17)
P(5)-F(6E)	1.613(14)	O(1A)-Ir(1)-P(2A)	98.06(18)
P(5)-F(3E)	1.616(15)	C(50A)-Ir(1)-P(2A)	84.4(2)
P(5)-F(2E)	1.652(14)	N(1A)-Ir(1)-P(2A)	93.78(18)
C(1L)-C(2L)	1.3900	O(2A)-Ir(1)-P(1A)	98.16(17)
C(1L)-C(6L)	1.3900	O(1A)-Ir(1)-P(1A)	81.81(18)
C(2L)-C(3L)	1.3900	C(50A)-Ir(1)-P(1A)	89.8(2)
C(3L)-C(4L)	1.3900	N(1A)-Ir(1)-P(1A)	91.96(18)
C(4L)-C(5L)	1.3900	P(2A)-Ir(1)-P(1A)	174.24(8)
C(5L)-C(6L)	1.3900	C(40A)-P(1A)-C(38A)	103.4(4)
P(6)-F(2F)	1.468(18)	C(40A)-P(1A)-C(42A)	103.5(4)

C(38A)-P(1A)-C(42A)	103.6(4)	N(1A)-C(7A)-C(8A)	117.4(7)
C(40A)-P(1A)-Ir(1)	114.9(3)	N(1A)-C(7A)-C(6A)	122.3(8)
C(38A)-P(1A)-Ir(1)	119.0(3)	C(8A)-C(7A)-C(6A)	120.2(8)
C(42A)-P(1A)-Ir(1)	110.7(3)	C(9A)-C(8A)-C(7A)	124.0(8)
C(48A)-P(2A)-C(44A)	104.7(5)	C(8A)-C(9A)-C(10A)	116.0(8)
C(48A)-P(2A)-C(46A)	103.3(4)	C(8A)-C(9A)-C(26A)	121.5(7)
C(44A)-P(2A)-C(46A)	105.6(4)	C(10A)-C(9A)-C(26A)	122.4(7)
C(48A)-P(2A)-Ir(1)	115.0(3)	C(11A)-C(10A)-C(9A)	119.5(8)
C(44A)-P(2A)-Ir(1)	108.9(3)	N(1A)-C(11A)-C(10A)	120.2(7)
C(46A)-P(2A)-Ir(1)	118.1(3)	N(1A)-C(11A)-C(12A)	123.3(7)
C(1A)-O(1A)-Ir(1)	118.4(5)	C(10A)-C(11A)-C(12A)	116.2(7)
C(17A)-O(2A)-Ir(1)	119.2(5)	C(13A)-C(12A)-C(17A)	119.2(7)
C(11A)-N(1A)-C(7A)	122.5(7)	C(13A)-C(12A)-C(11A)	118.0(7)
C(11A)-N(1A)-Ir(1)	118.0(5)	C(17A)-C(12A)-C(11A)	122.5(7)
C(7A)-N(1A)-Ir(1)	119.4(5)	C(14A)-C(13A)-C(12A)	121.5(8)
O(1A)-C(1A)-C(6A)	121.9(8)	C(13A)-C(14A)-C(15A)	118.2(8)
O(1A)-C(1A)-C(2A)	117.9(8)	C(13A)-C(14A)-C(30A)	119.7(7)
C(6A)-C(1A)-C(2A)	120.1(8)	C(15A)-C(14A)-C(30A)	122.1(7)
C(3A)-C(2A)-C(1A)	117.1(8)	C(16A)-C(15A)-C(14A)	124.0(8)
C(3A)-C(2A)-C(18A)	121.2(8)	C(15A)-C(16A)-C(17A)	116.8(8)
C(1A)-C(2A)-C(18A)	121.7(8)	C(15A)-C(16A)-C(34A)	122.7(8)
C(2A)-C(3A)-C(4A)	123.3(8)	C(17A)-C(16A)-C(34A)	120.2(8)
C(5A)-C(4A)-C(3A)	117.6(8)	O(2A)-C(17A)-C(12A)	120.7(7)
C(5A)-C(4A)-C(22A)	124.0(8)	O(2A)-C(17A)-C(16A)	120.4(8)
C(3A)-C(4A)-C(22A)	118.4(8)	C(12A)-C(17A)-C(16A)	118.7(8)
C(4A)-C(5A)-C(6A)	122.7(8)	C(20A)-C(18A)-C(21A)	107.4(8)
C(1A)-C(6A)-C(5A)	118.2(8)	C(20A)-C(18A)-C(2A)	113.1(7)
C(1A)-C(6A)-C(7A)	124.9(8)	C(21A)-C(18A)-C(2A)	112.7(8)
C(5A)-C(6A)-C(7A)	116.9(8)	C(20A)-C(18A)-C(19A)	110.8(8)

C(21A)-C(18A)-C(19A)	106.4(8)	C(45A)-C(44A)-P(2A)	117.9(7)
C(2A)-C(18A)-C(19A)	106.3(8)	C(47A)-C(46A)-P(2A)	115.4(6)
C(23A)-C(22A)-C(24A)	111.4(7)	C(49A)-C(48A)-P(2A)	119.9(7)
C(23A)-C(22A)-C(25A)	105.9(7)	O(2B)-Ir(2)-O(1B)	173.4(2)
C(24A)-C(22A)-C(25A)	107.0(7)	O(2B)-Ir(2)-N(1B)	86.3(2)
C(23A)-C(22A)-C(4A)	112.5(7)	O(1B)-Ir(2)-N(1B)	87.1(2)
C(24A)-C(22A)-C(4A)	108.8(7)	O(2B)-Ir(2)-C(50B)	95.6(3)
C(25A)-C(22A)-C(4A)	111.2(7)	O(1B)-Ir(2)-C(50B)	91.0(3)
C(27A)-C(26A)-C(29A)	110.9(7)	N(1B)-Ir(2)-C(50B)	177.1(3)
C(27A)-C(26A)-C(9A)	108.8(7)	O(2B)-Ir(2)-P(2B)	82.09(17)
C(29A)-C(26A)-C(9A)	112.2(7)	O(1B)-Ir(2)-P(2B)	98.13(17)
C(27A)-C(26A)-C(28A)	109.4(7)	N(1B)-Ir(2)-P(2B)	93.62(19)
C(29A)-C(26A)-C(28A)	109.7(7)	C(50B)-Ir(2)-P(2B)	84.5(2)
C(9A)-C(26A)-C(28A)	105.7(7)	O(2B)-Ir(2)-P(1B)	98.47(17)
C(32A)-C(30A)-C(31A)	107.8(7)	O(1B)-Ir(2)-P(1B)	82.05(17)
C(32A)-C(30A)-C(33A)	110.2(7)	N(1B)-Ir(2)-P(1B)	92.72(19)
C(31A)-C(30A)-C(33A)	108.6(7)	C(50B)-Ir(2)-P(1B)	89.2(2)
C(32A)-C(30A)-C(14A)	112.8(7)	P(2B)-Ir(2)-P(1B)	173.65(8)
C(31A)-C(30A)-C(14A)	110.0(7)	C(42B)-P(1B)-C(38B)	102.7(4)
C(33A)-C(30A)-C(14A)	107.5(7)	C(42B)-P(1B)-C(40B)	102.6(4)
C(35A)-C(34A)-C(37A)	110.8(8)	C(38B)-P(1B)-C(40B)	104.4(4)
C(35A)-C(34A)-C(16A)	110.6(8)	C(42B)-P(1B)-Ir(2)	116.1(3)
C(37A)-C(34A)-C(16A)	111.1(7)	C(38B)-P(1B)-Ir(2)	117.6(3)
C(35A)-C(34A)-C(36A)	108.8(7)	C(40B)-P(1B)-Ir(2)	111.7(3)
C(37A)-C(34A)-C(36A)	106.0(7)	C(46B)-P(2B)-C(44B)	103.3(4)
C(16A)-C(34A)-C(36A)	109.3(7)	C(46B)-P(2B)-C(48B)	105.8(4)
C(39A)-C(38A)-P(1A)	115.3(6)	C(44B)-P(2B)-C(48B)	103.3(4)
C(41A)-C(40A)-P(1A)	117.1(6)	C(46B)-P(2B)-Ir(2)	117.1(3)
C(43A)-C(42A)-P(1A)	114.9(6)	C(44B)-P(2B)-Ir(2)	111.0(3)

C(48B)-P(2B)-Ir(2)	114.9(3)	N(1B)-C(11B)-C(12B)	120.7(8)
C(1B)-O(1B)-Ir(2)	120.6(5)	C(10B)-C(11B)-C(12B)	120.6(8)
C(17B)-O(2B)-Ir(2)	120.2(5)	C(17B)-C(12B)-C(13B)	119.1(8)
C(11B)-N(1B)-C(7B)	119.8(7)	C(17B)-C(12B)-C(11B)	123.4(8)
C(11B)-N(1B)-Ir(2)	120.8(6)	C(13B)-C(12B)-C(11B)	116.4(8)
C(7B)-N(1B)-Ir(2)	119.3(5)	C(14B)-C(13B)-C(12B)	122.3(8)
O(1B)-C(1B)-C(2B)	119.8(7)	C(13B)-C(14B)-C(15B)	117.8(8)
O(1B)-C(1B)-C(6B)	119.3(7)	C(13B)-C(14B)-C(30B)	118.9(8)
C(2B)-C(1B)-C(6B)	120.9(8)	C(15B)-C(14B)-C(30B)	122.9(7)
C(3B)-C(2B)-C(1B)	116.3(8)	C(14B)-C(15B)-C(16B)	123.7(8)
C(3B)-C(2B)-C(18B)	121.7(7)	C(15B)-C(16B)-C(17B)	117.1(8)
C(1B)-C(2B)-C(18B)	121.9(8)	C(15B)-C(16B)-C(34B)	120.8(7)
C(2B)-C(3B)-C(4B)	124.8(8)	C(17B)-C(16B)-C(34B)	122.0(7)
C(5B)-C(4B)-C(3B)	118.2(8)	O(2B)-C(17B)-C(12B)	121.6(8)
C(5B)-C(4B)-C(22B)	120.2(8)	O(2B)-C(17B)-C(16B)	118.7(7)
C(3B)-C(4B)-C(22B)	121.3(8)	C(12B)-C(17B)-C(16B)	119.6(8)
C(4B)-C(5B)-C(6B)	122.1(8)	C(2B)-C(18B)-C(19B)	109.7(7)
C(1B)-C(6B)-C(5B)	117.2(7)	C(2B)-C(18B)-C(21B)	113.6(7)
C(1B)-C(6B)-C(7B)	124.4(8)	C(19B)-C(18B)-C(21B)	108.1(7)
C(5B)-C(6B)-C(7B)	117.7(7)	C(2B)-C(18B)-C(20B)	111.4(7)
N(1B)-C(7B)-C(8B)	119.7(8)	C(19B)-C(18B)-C(20B)	108.7(7)
N(1B)-C(7B)-C(6B)	120.8(7)	C(21B)-C(18B)-C(20B)	105.2(7)
C(8B)-C(7B)-C(6B)	119.5(8)	C(4B)-C(22B)-C(25B)	113.7(8)
C(7B)-C(8B)-C(9B)	121.7(8)	C(4B)-C(22B)-C(24B)	110.1(7)
C(10B)-C(9B)-C(8B)	116.1(8)	C(25B)-C(22B)-C(24B)	110.4(8)
C(10B)-C(9B)-C(26B)	125.1(8)	C(4B)-C(22B)-C(23B)	107.4(8)
C(8B)-C(9B)-C(26B)	118.8(8)	C(25B)-C(22B)-C(23B)	109.4(8)
C(9B)-C(10B)-C(11B)	123.6(8)	C(24B)-C(22B)-C(23B)	105.4(8)
N(1B)-C(11B)-C(10B)	118.6(8)	C(27B)-C(26B)-C(9B)	111.6(7)

C(27B)-C(26B)-C(29B)	107.5(7)	O(2C)-Ir(3)-P(2C)	97.05(19)
C(9B)-C(26B)-C(29B)	111.5(7)	O(1C)-Ir(3)-P(2C)	83.01(18)
C(27B)-C(26B)-C(28B)	111.3(8)	N(1C)-Ir(3)-P(2C)	93.64(19)
C(9B)-C(26B)-C(28B)	106.1(7)	C(50C)-Ir(3)-P(2C)	84.7(2)
C(29B)-C(26B)-C(28B)	108.8(7)	O(2C)-Ir(3)-P(1C)	80.95(19)
C(31B)-C(30B)-C(33B)	110.0(7)	O(1C)-Ir(3)-P(1C)	99.94(18)
C(31B)-C(30B)-C(32B)	107.8(7)	N(1C)-Ir(3)-P(1C)	94.24(19)
C(33B)-C(30B)-C(32B)	108.8(7)	C(50C)-Ir(3)-P(1C)	87.5(2)
C(31B)-C(30B)-C(14B)	110.5(7)	P(2C)-Ir(3)-P(1C)	171.73(9)
C(33B)-C(30B)-C(14B)	107.9(7)	C(38C)-P(1C)-C(40C)	107.2(4)
C(32B)-C(30B)-C(14B)	111.8(7)	C(38C)-P(1C)-C(42C)	105.0(4)
C(35B)-C(34B)-C(37B)	112.0(7)	C(40C)-P(1C)-C(42C)	103.4(4)
C(35B)-C(34B)-C(36B)	107.7(7)	C(38C)-P(1C)-Ir(3)	109.5(3)
C(37B)-C(34B)-C(36B)	104.7(7)	C(40C)-P(1C)-Ir(3)	115.9(3)
C(35B)-C(34B)-C(16B)	106.7(7)	C(42C)-P(1C)-Ir(3)	114.9(3)
C(37B)-C(34B)-C(16B)	112.3(7)	C(46C)-P(2C)-C(48C)	103.7(4)
C(36B)-C(34B)-C(16B)	113.6(7)	C(46C)-P(2C)-C(44C)	107.3(4)
C(39B)-C(38B)-P(1B)	113.1(6)	C(48C)-P(2C)-C(44C)	102.3(4)
C(41B)-C(40B)-P(1B)	115.5(6)	C(46C)-P(2C)-Ir(3)	117.2(3)
C(43B)-C(42B)-P(1B)	116.4(6)	C(48C)-P(2C)-Ir(3)	112.5(3)
C(45B)-C(44B)-P(2B)	118.0(7)	C(44C)-P(2C)-Ir(3)	112.5(3)
C(47B)-C(46B)-P(2B)	113.8(6)	C(1C)-O(1C)-Ir(3)	118.3(5)
C(49B)-C(48B)-P(2B)	115.8(6)	C(17C)-O(2C)-Ir(3)	120.5(5)
O(2C)-Ir(3)-O(1C)	173.2(2)	C(11C)-N(1C)-C(7C)	121.6(7)
O(2C)-Ir(3)-N(1C)	86.6(3)	C(11C)-N(1C)-Ir(3)	119.4(6)
O(1C)-Ir(3)-N(1C)	86.6(2)	C(7C)-N(1C)-Ir(3)	118.9(5)
O(2C)-Ir(3)-C(50C)	94.1(3)	O(1C)-C(1C)-C(2C)	120.8(8)
O(1C)-Ir(3)-C(50C)	92.7(3)	O(1C)-C(1C)-C(6C)	121.5(8)
N(1C)-Ir(3)-C(50C)	178.3(3)	C(2C)-C(1C)-C(6C)	117.7(9)

C(3C)-C(2C)-C(1C)	119.4(9)	C(16C)-C(15C)-C(14C)	124.0(9)
C(3C)-C(2C)-C(18C)	119.6(9)	C(15C)-C(16C)-C(17C)	115.8(8)
C(1C)-C(2C)-C(18C)	120.9(9)	C(15C)-C(16C)-C(34C)	123.4(8)
C(2C)-C(3C)-C(4C)	121.9(10)	C(17C)-C(16C)-C(34C)	120.7(8)
C(5C)-C(4C)-C(3C)	118.2(10)	O(2C)-C(17C)-C(12C)	121.8(8)
C(5C)-C(4C)-C(22C)	123.0(10)	O(2C)-C(17C)-C(16C)	117.8(8)
C(3C)-C(4C)-C(22C)	118.7(10)	C(12C)-C(17C)-C(16C)	120.4(8)
C(6C)-C(5C)-C(4C)	121.2(10)	C(2C)-C(18C)-C(21C)	112.7(9)
C(5C)-C(6C)-C(1C)	120.9(9)	C(2C)-C(18C)-C(20C)	108.1(8)
C(5C)-C(6C)-C(7C)	117.5(8)	C(21C)-C(18C)-C(20C)	107.9(9)
C(1C)-C(6C)-C(7C)	121.2(8)	C(2C)-C(18C)-C(19C)	110.7(8)
N(1C)-C(7C)-C(8C)	118.1(8)	C(21C)-C(18C)-C(19C)	109.2(8)
N(1C)-C(7C)-C(6C)	121.4(7)	C(20C)-C(18C)-C(19C)	108.1(8)
C(8C)-C(7C)-C(6C)	120.5(8)	C(23C)-C(22C)-C(24C)	115.7(14)
C(9C)-C(8C)-C(7C)	124.1(9)	C(23C)-C(22C)-C(25C)	104.4(11)
C(8C)-C(9C)-C(10C)	115.5(9)	C(24C)-C(22C)-C(25C)	106.3(11)
C(8C)-C(9C)-C(26C)	121.4(9)	C(23C)-C(22C)-C(4C)	108.4(14)
C(10C)-C(9C)-C(26C)	123.0(8)	C(24C)-C(22C)-C(4C)	109.3(15)
C(9C)-C(10C)-C(11C)	122.9(8)	C(25C)-C(22C)-C(4C)	112.7(10)
N(1C)-C(11C)-C(10C)	117.7(8)	C(29C)-C(26C)-C(9C)	113.6(9)
N(1C)-C(11C)-C(12C)	122.8(8)	C(29C)-C(26C)-C(28C)	113.4(10)
C(10C)-C(11C)-C(12C)	119.6(8)	C(9C)-C(26C)-C(28C)	108.7(9)
C(13C)-C(12C)-C(17C)	117.7(8)	C(29C)-C(26C)-C(27C)	106.7(9)
C(13C)-C(12C)-C(11C)	119.5(8)	C(9C)-C(26C)-C(27C)	108.3(8)
C(17C)-C(12C)-C(11C)	122.0(8)	C(28C)-C(26C)-C(27C)	105.7(9)
C(14C)-C(13C)-C(12C)	123.7(8)	C(33C)-C(30C)-C(14C)	112.8(8)
C(13C)-C(14C)-C(15C)	118.1(9)	C(33C)-C(30C)-C(32C)	108.9(8)
C(13C)-C(14C)-C(30C)	122.4(8)	C(14C)-C(30C)-C(32C)	107.4(8)
C(15C)-C(14C)-C(30C)	119.5(8)	C(33C)-C(30C)-C(31C)	109.4(8)

C(14C)-C(30C)-C(31C)	109.1(7)	C(38D)-P(1D)-C(40D)	104.8(5)
C(32C)-C(30C)-C(31C)	109.2(8)	C(38D)-P(1D)-C(42D)	104.6(5)
C(35C)-C(34C)-C(37C)	111.7(8)	C(40D)-P(1D)-C(42D)	105.9(5)
C(35C)-C(34C)-C(16C)	108.1(7)	C(38D)-P(1D)-Ir(4)	109.6(3)
C(37C)-C(34C)-C(16C)	111.9(7)	C(40D)-P(1D)-Ir(4)	115.4(4)
C(35C)-C(34C)-C(36C)	108.6(8)	C(42D)-P(1D)-Ir(4)	115.5(3)
C(37C)-C(34C)-C(36C)	109.4(8)	C(46D)-P(2D)-C(48D)	103.1(5)
C(16C)-C(34C)-C(36C)	107.0(8)	C(46D)-P(2D)-C(44D)	109.0(4)
C(39C)-C(38C)-P(1C)	118.0(7)	C(48D)-P(2D)-C(44D)	104.1(5)
C(41C)-C(40C)-P(1C)	115.9(7)	C(46D)-P(2D)-Ir(4)	116.2(3)
C(43C)-C(42C)-P(1C)	115.1(7)	C(48D)-P(2D)-Ir(4)	112.4(3)
C(45C)-C(44C)-P(2C)	115.9(7)	C(44D)-P(2D)-Ir(4)	111.1(4)
C(47C)-C(46C)-P(2C)	112.0(6)	C(1D)-O(1D)-Ir(4)	118.8(6)
C(49C)-C(48C)-P(2C)	113.0(6)	C(17D)-O(2D)-Ir(4)	121.8(6)
O(1D)-Ir(4)-O(2D)	172.1(2)	C(11D)-N(1D)-C(7D)	120.6(7)
O(1D)-Ir(4)-C(50D)	93.3(3)	C(11D)-N(1D)-Ir(4)	120.8(6)
O(2D)-Ir(4)-C(50D)	94.6(3)	C(7D)-N(1D)-Ir(4)	118.5(6)
O(1D)-Ir(4)-N(1D)	86.8(3)	O(1D)-C(1D)-C(6D)	119.9(8)
O(2D)-Ir(4)-N(1D)	85.3(3)	O(1D)-C(1D)-C(2D)	120.0(9)
C(50D)-Ir(4)-N(1D)	178.8(3)	C(6D)-C(1D)-C(2D)	120.0(9)
O(1D)-Ir(4)-P(2D)	82.83(19)	C(3D)-C(2D)-C(1D)	117.7(9)
O(2D)-Ir(4)-P(2D)	97.0(2)	C(3D)-C(2D)-C(18D)	122.0(9)
C(50D)-Ir(4)-P(2D)	86.8(3)	C(1D)-C(2D)-C(18D)	120.4(9)
N(1D)-Ir(4)-P(2D)	94.3(2)	C(2D)-C(3D)-C(4D)	123.6(9)
O(1D)-Ir(4)-P(1D)	99.65(19)	C(3D)-C(4D)-C(5D)	118.3(9)
O(2D)-Ir(4)-P(1D)	81.6(2)	C(3D)-C(4D)-C(22D)	119.6(9)
C(50D)-Ir(4)-P(1D)	85.7(3)	C(5D)-C(4D)-C(22D)	121.9(9)
N(1D)-Ir(4)-P(1D)	93.1(2)	C(4D)-C(5D)-C(6D)	120.2(9)
P(2D)-Ir(4)-P(1D)	172.30(9)	C(1D)-C(6D)-C(5D)	119.0(8)

C(1D)-C(6D)-C(7D)	123.9(9)	C(21D)-C(18D)-C(19D)	108.3(8)
C(5D)-C(6D)-C(7D)	116.6(8)	C(20D)-C(18D)-C(2D)	108.0(8)
N(1D)-C(7D)-C(8D)	120.2(8)	C(21D)-C(18D)-C(2D)	112.4(9)
N(1D)-C(7D)-C(6D)	120.5(8)	C(19D)-C(18D)-C(2D)	111.4(8)
C(8D)-C(7D)-C(6D)	119.1(8)	C(23D)-C(22D)-C(25D)	109.6(10)
C(9D)-C(8D)-C(7D)	120.4(8)	C(23D)-C(22D)-C(24D)	107.0(9)
C(10D)-C(9D)-C(8D)	118.2(8)	C(25D)-C(22D)-C(24D)	108.1(9)
C(10D)-C(9D)-C(26D)	122.5(9)	C(23D)-C(22D)-C(4D)	110.6(9)
C(8D)-C(9D)-C(26D)	119.2(8)	C(25D)-C(22D)-C(4D)	112.4(9)
C(9D)-C(10D)-C(11D)	120.9(8)	C(24D)-C(22D)-C(4D)	109.0(8)
N(1D)-C(11D)-C(10D)	119.4(8)	C(29D)-C(26D)-C(9D)	115.0(8)
N(1D)-C(11D)-C(12D)	121.0(8)	C(29D)-C(26D)-C(27D)	112.4(9)
C(10D)-C(11D)-C(12D)	119.4(8)	C(9D)-C(26D)-C(27D)	110.2(9)
C(13D)-C(12D)-C(17D)	116.4(8)	C(29D)-C(26D)-C(28D)	105.2(8)
C(13D)-C(12D)-C(11D)	117.7(8)	C(9D)-C(26D)-C(28D)	108.7(8)
C(17D)-C(12D)-C(11D)	125.7(8)	C(27D)-C(26D)-C(28D)	104.6(8)
C(14D)-C(13D)-C(12D)	122.3(8)	C(31D)-C(30D)-C(32D)	108.3(9)
C(15D)-C(14D)-C(13D)	118.3(9)	C(31D)-C(30D)-C(33D)	102.7(9)
C(15D)-C(14D)-C(30D)	120.4(8)	C(32D)-C(30D)-C(33D)	112.0(9)
C(13D)-C(14D)-C(30D)	121.3(8)	C(31D)-C(30D)-C(14D)	109.4(8)
C(14D)-C(15D)-C(16D)	123.1(9)	C(32D)-C(30D)-C(14D)	110.4(8)
C(15D)-C(16D)-C(17D)	118.9(9)	C(33D)-C(30D)-C(14D)	113.6(8)
C(15D)-C(16D)-C(34D)	120.2(8)	C(36D)-C(34D)-C(37D)	105.0(8)
C(17D)-C(16D)-C(34D)	120.9(8)	C(36D)-C(34D)-C(35D)	110.8(9)
O(2D)-C(17D)-C(16D)	121.2(8)	C(37D)-C(34D)-C(35D)	108.8(9)
O(2D)-C(17D)-C(12D)	118.7(8)	C(36D)-C(34D)-C(16D)	112.3(8)
C(16D)-C(17D)-C(12D)	120.0(9)	C(37D)-C(34D)-C(16D)	113.4(8)
C(20D)-C(18D)-C(21D)	106.3(8)	C(35D)-C(34D)-C(16D)	106.7(8)
C(20D)-C(18D)-C(19D)	110.3(9)	C(39D)-C(38D)-P(1D)	117.1(7)

C(41D)-C(40D)-P(1D)	116.4(7)	F(1A)-P(1)-F(5A)	96.5(10)
C(43D)-C(42D)-P(1D)	113.7(7)	F(1A)-P(1)-F(2A)	91.9(9)
C(45D)-C(44D)-P(2D)	120.0(8)	F(5A)-P(1)-F(2A)	90.9(10)
C(47D)-C(46D)-P(2D)	115.7(6)	F(1A)-P(1)-F(6A)	95.0(9)
C(49D)-C(48D)-P(2D)	115.4(7)	F(5A)-P(1)-F(6A)	168.2(11)
C(2E)-C(1E)-C(3E)#1	116.5(10)	F(2A)-P(1)-F(6A)	86.0(10)
C(3E)-C(2E)-C(1E)	122.9(10)	F(1A)-P(1)-F(4A)	92.7(9)
C(2E)-C(3E)-C(1E)#1	120.5(10)	F(5A)-P(1)-F(4A)	88.7(10)
C(2F)-C(1F)-C(3F)#2	120.3(11)	F(2A)-P(1)-F(4A)	175.4(10)
C(1F)-C(2F)-C(3F)	118.6(10)	F(6A)-P(1)-F(4A)	93.5(9)
C(2F)-C(3F)-C(1F)#2	121.1(11)	F(1A)-P(1)-F(3A)	172.5(10)
C(2G)-C(1G)-C(6G)	120.0	F(5A)-P(1)-F(3A)	89.4(9)
C(3G)-C(2G)-C(1G)	120.0	F(2A)-P(1)-F(3A)	92.6(9)
C(2G)-C(3G)-C(4G)	120.0	F(6A)-P(1)-F(3A)	79.4(9)
C(5G)-C(4G)-C(3G)	120.0	F(4A)-P(1)-F(3A)	82.8(8)
C(6G)-C(5G)-C(4G)	120.0	C(2J)-C(1J)-C(6J)	120.0
C(5G)-C(6G)-C(1G)	120.0	C(1J)-C(2J)-C(3J)	120.0
C(2H)-C(1H)-C(6H)	120.0	C(2J)-C(3J)-C(4J)	120.0
C(1H)-C(2H)-C(3H)	120.0	C(5J)-C(4J)-C(3J)	120.0
C(4H)-C(3H)-C(2H)	120.0	C(6J)-C(5J)-C(4J)	120.0
C(5H)-C(4H)-C(3H)	120.0	C(5J)-C(6J)-C(1J)	120.0
C(6H)-C(5H)-C(4H)	120.0	F(1B)-P(2)-F(3B)	91.7(3)
C(5H)-C(6H)-C(1H)	120.0	F(1B)-P(2)-F(6B)	90.1(3)
C(2I)-C(1I)-C(6I)	120.0	F(3B)-P(2)-F(6B)	90.9(3)
C(3I)-C(2I)-C(1I)	120.0	F(1B)-P(2)-F(4B)	90.7(3)
C(2I)-C(3I)-C(4I)	120.0	F(3B)-P(2)-F(4B)	89.2(3)
C(3I)-C(4I)-C(5I)	120.0	F(6B)-P(2)-F(4B)	179.1(4)
C(6I)-C(5I)-C(4I)	120.0	F(1B)-P(2)-F(5B)	88.0(4)
C(5I)-C(6I)-C(1I)	120.0	F(3B)-P(2)-F(5B)	178.5(4)

F(6B)-P(2)-F(5B)	90.6(4)	F(4D)-P(4)-F(2D)	177.9(6)
F(4B)-P(2)-F(5B)	89.3(3)	F(6D)-P(4)-F(2D)	89.6(6)
F(1B)-P(2)-F(2B)	178.1(4)	F(1D)-P(4)-F(2D)	84.0(5)
F(3B)-P(2)-F(2B)	89.6(3)	F(5D)-P(4)-F(3D)	89.0(6)
F(6B)-P(2)-F(2B)	88.5(3)	F(4D)-P(4)-F(3D)	90.8(6)
F(4B)-P(2)-F(2B)	90.7(3)	F(6D)-P(4)-F(3D)	177.6(6)
F(5B)-P(2)-F(2B)	90.7(4)	F(1D)-P(4)-F(3D)	88.6(5)
F(5C)-P(3)-F(3C)	91.0(4)	F(2D)-P(4)-F(3D)	88.0(5)
F(5C)-P(3)-F(6C)	90.0(3)	C(2K)-C(1K)-C(6K)	120.0
F(3C)-P(3)-F(6C)	177.4(4)	C(3K)-C(2K)-C(1K)	120.0
F(5C)-P(3)-F(4C)	177.4(4)	C(4K)-C(3K)-C(2K)	120.0
F(3C)-P(3)-F(4C)	91.6(3)	C(3K)-C(4K)-C(5K)	120.0
F(6C)-P(3)-F(4C)	87.3(3)	C(6K)-C(5K)-C(4K)	120.0
F(5C)-P(3)-F(1C)	88.5(3)	C(5K)-C(6K)-C(1K)	120.0
F(3C)-P(3)-F(1C)	91.0(3)	F(4E)-P(5)-F(1E)	93.9(7)
F(6C)-P(3)-F(1C)	86.6(3)	F(4E)-P(5)-F(5E)	89.3(7)
F(4C)-P(3)-F(1C)	91.5(3)	F(1E)-P(5)-F(5E)	87.9(7)
F(5C)-P(3)-F(2C)	90.3(3)	F(4E)-P(5)-F(6E)	88.2(7)
F(3C)-P(3)-F(2C)	89.3(3)	F(1E)-P(5)-F(6E)	176.1(8)
F(6C)-P(3)-F(2C)	93.1(3)	F(5E)-P(5)-F(6E)	88.9(7)
F(4C)-P(3)-F(2C)	89.7(3)	F(4E)-P(5)-F(3E)	95.0(8)
F(1C)-P(3)-F(2C)	178.8(4)	F(1E)-P(5)-F(3E)	95.4(7)
F(5D)-P(4)-F(4D)	91.2(6)	F(5E)-P(5)-F(3E)	174.4(8)
F(5D)-P(4)-F(6D)	91.4(6)	F(6E)-P(5)-F(3E)	87.7(7)
F(4D)-P(4)-F(6D)	91.5(5)	F(4E)-P(5)-F(2E)	176.2(8)
F(5D)-P(4)-F(1D)	174.1(6)	F(1E)-P(5)-F(2E)	88.9(7)
F(4D)-P(4)-F(1D)	94.3(5)	F(5E)-P(5)-F(2E)	88.3(7)
F(6D)-P(4)-F(1D)	90.8(5)	F(6E)-P(5)-F(2E)	88.8(7)
F(5D)-P(4)-F(2D)	90.5(6)	F(3E)-P(5)-F(2E)	87.2(7)

C(2L)-C(1L)-C(6L)	120.0
C(3L)-C(2L)-C(1L)	120.0
C(4L)-C(3L)-C(2L)	120.0
C(5L)-C(4L)-C(3L)	120.0
C(4L)-C(5L)-C(6L)	120.0
C(5L)-C(6L)-C(1L)	120.0
F(2F)-P(6)-F(5F)	99.1(11)
F(2F)-P(6)-F(4F)	166.6(13)
F(5F)-P(6)-F(4F)	85.5(11)
F(2F)-P(6)-F(6F)	105.2(12)
F(5F)-P(6)-F(6F)	92.8(12)
F(4F)-P(6)-F(6F)	87.0(12)
F(2F)-P(6)-F(3F)	92.5(11)
F(5F)-P(6)-F(3F)	159.8(11)
F(4F)-P(6)-F(3F)	79.7(10)
F(6F)-P(6)-F(3F)	100.0(11)
F(2F)-P(6)-F(1F)	88.3(10)
F(5F)-P(6)-F(1F)	79.1(11)
F(4F)-P(6)-F(1F)	80.2(10)
F(6F)-P(6)-F(1F)	165.3(12)
F(3F)-P(6)-F(1F)	84.8(9)
C(2M)-C(1M)-C(6M)	120.0
C(1M)-C(2M)-C(3M)	120.0
C(4M)-C(3M)-C(2M)	120.0
C(5M)-C(4M)-C(3M)	120.0
C(4M)-C(5M)-C(6M)	120.0
C(5M)-C(6M)-C(1M)	120.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z

#2 -x+1,-y+1,-z

Table S57. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **16**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	100(2)	289(2)	109(2)	-54(2)	-16(2)	12(2)
P(1A)	114(13)	276(14)	123(12)	-30(11)	-1(10)	11(11)
P(2A)	185(14)	308(15)	134(13)	-77(11)	-2(11)	-45(11)
O(1A)	160(30)	210(30)	240(30)	-20(20)	20(30)	-10(20)
O(2A)	210(30)	200(30)	120(30)	-30(20)	-20(20)	30(20)
N(1A)	70(18)	77(18)	69(18)	3(10)	-6(10)	10(10)
C(1A)	120(40)	200(40)	110(30)	20(30)	-10(30)	-20(30)
C(2A)	160(40)	170(40)	150(40)	-40(30)	-10(30)	-40(30)
C(3A)	180(40)	220(40)	110(30)	-70(30)	-20(30)	-20(30)
C(4A)	200(40)	230(40)	160(40)	-30(30)	0(30)	-20(30)
C(5A)	140(40)	200(40)	140(40)	-50(30)	0(30)	-10(30)
C(6A)	180(40)	190(40)	140(40)	0(30)	-50(30)	10(30)
C(7A)	130(40)	180(40)	80(30)	-30(30)	70(30)	-20(30)
C(8A)	70(40)	160(40)	150(40)	10(30)	0(30)	60(30)
C(9A)	140(40)	180(40)	90(30)	30(30)	0(30)	20(30)
C(10A)	160(40)	200(40)	160(40)	-50(30)	-40(30)	50(30)
C(11A)	50(40)	160(40)	120(40)	-10(30)	0(30)	0(30)
C(12A)	80(40)	170(40)	160(40)	-60(30)	-50(30)	10(30)
C(13A)	130(40)	170(40)	150(40)	-20(30)	-30(30)	20(30)
C(14A)	160(40)	180(40)	160(40)	-30(30)	-20(30)	20(30)

C(15A)	180(40)	150(40)	240(40)	-30(30)	-30(30)	50(30)
C(16A)	170(40)	210(40)	170(40)	40(30)	-50(30)	-20(30)
C(17A)	190(40)	180(40)	150(40)	0(30)	10(30)	30(30)
C(18A)	230(40)	260(40)	290(40)	-10(30)	20(30)	20(30)
C(19A)	370(50)	400(40)	370(40)	-90(40)	70(40)	-60(40)
C(20A)	220(40)	320(40)	320(40)	-120(30)	-90(30)	-60(30)
C(21A)	320(40)	340(40)	370(40)	-90(40)	10(40)	-60(40)
C(22A)	160(40)	230(40)	240(40)	0(30)	-60(30)	50(30)
C(23A)	300(40)	310(40)	350(40)	-100(30)	40(40)	50(30)
C(24A)	400(50)	390(40)	460(50)	-70(40)	-70(40)	110(40)
C(25A)	430(50)	530(50)	590(50)	-120(40)	10(40)	80(40)
C(26A)	80(40)	180(40)	50(30)	20(30)	-30(30)	0(30)
C(27A)	280(40)	310(40)	250(40)	-30(30)	-100(30)	-20(30)
C(28A)	230(40)	390(40)	240(40)	-20(30)	10(30)	-10(30)
C(29A)	180(40)	290(40)	250(40)	-40(30)	-50(30)	30(30)
C(30A)	210(40)	150(40)	240(40)	-50(30)	-10(30)	50(30)
C(31A)	240(40)	290(40)	300(40)	-120(30)	20(30)	0(30)
C(32A)	470(50)	400(40)	390(40)	-80(40)	0(40)	70(40)
C(33A)	250(40)	330(40)	280(40)	-50(30)	10(30)	90(30)
C(34A)	280(40)	250(40)	240(40)	-10(30)	-50(30)	20(30)
C(35A)	290(40)	350(40)	300(40)	0(30)	-60(40)	-50(40)
C(36A)	350(40)	360(40)	300(40)	-10(30)	-200(40)	-10(40)
C(37A)	250(40)	330(40)	240(40)	40(30)	-50(30)	0(30)
C(38A)	150(40)	230(40)	180(40)	-20(30)	-10(30)	10(30)
C(39A)	240(40)	350(40)	320(40)	-40(30)	40(30)	40(30)
C(40A)	160(40)	250(40)	140(40)	-80(30)	0(30)	20(30)
C(41A)	160(40)	260(40)	190(40)	10(30)	-20(30)	-10(30)
C(42A)	160(40)	210(40)	180(40)	-40(30)	0(30)	-10(30)
C(43A)	180(40)	220(40)	220(40)	-70(30)	0(30)	-80(30)

C(44A)	250(40)	420(40)	230(40)	40(30)	0(30)	30(40)
C(45A)	350(40)	410(40)	240(40)	30(30)	10(30)	40(40)
C(46A)	160(40)	270(40)	200(40)	0(30)	-10(30)	-30(30)
C(47A)	190(40)	240(40)	160(40)	-20(30)	-30(30)	-80(30)
C(48A)	250(40)	270(40)	230(40)	-110(30)	0(30)	-50(30)
C(49A)	570(50)	500(50)	600(50)	-210(40)	210(40)	-60(40)
C(50A)	200(40)	320(40)	210(40)	-50(30)	-30(30)	-40(30)
Ir(2)	124(2)	189(2)	114(2)	-21(2)	-4(2)	7(2)
P(1B)	126(13)	188(13)	126(12)	-16(10)	13(10)	4(10)
P(2B)	166(13)	194(13)	121(12)	-3(10)	27(10)	17(11)
O(1B)	110(30)	170(30)	180(30)	-50(20)	-30(20)	-20(20)
O(2B)	180(30)	150(30)	120(30)	20(20)	0(20)	-20(20)
N(1B)	210(30)	110(30)	80(30)	20(30)	-20(30)	-10(30)
C(1B)	110(40)	170(40)	180(40)	-30(30)	10(30)	0(30)
C(2B)	100(40)	160(40)	120(40)	-20(30)	-30(30)	0(30)
C(3B)	170(40)	140(40)	150(40)	-10(30)	40(30)	0(30)
C(4B)	140(40)	170(40)	120(30)	-10(30)	30(30)	-30(30)
C(5B)	120(40)	200(40)	190(40)	-20(30)	-10(30)	100(30)
C(6B)	120(40)	140(40)	100(30)	10(30)	-50(30)	0(30)
C(7B)	110(40)	210(40)	150(40)	-60(30)	-10(30)	30(30)
C(8B)	140(40)	170(40)	150(40)	0(30)	-40(30)	-10(30)
C(9B)	120(40)	200(40)	90(30)	-60(30)	10(30)	0(30)
C(10B)	110(40)	140(40)	110(30)	0(30)	40(30)	60(30)
C(11B)	180(40)	140(40)	200(40)	-110(30)	50(30)	40(30)
C(12B)	120(40)	120(30)	120(30)	40(30)	20(30)	30(30)
C(13B)	180(40)	180(40)	140(40)	-30(30)	-50(30)	30(30)
C(14B)	100(40)	130(40)	150(40)	20(30)	-30(30)	50(30)
C(15B)	120(40)	130(30)	190(40)	-10(30)	-50(30)	-10(30)

C(16B)	160(40)	210(40)	180(40)	-50(30)	20(30)	10(30)
C(17B)	110(40)	190(40)	120(40)	-10(30)	-30(30)	60(30)
C(18B)	200(40)	190(40)	180(40)	0(30)	-20(30)	10(30)
C(19B)	170(40)	250(40)	260(40)	-20(30)	-20(30)	80(30)
C(20B)	270(40)	250(40)	310(40)	-70(30)	-30(30)	10(30)
C(21B)	210(40)	240(40)	370(40)	10(30)	-40(30)	20(30)
C(22B)	250(40)	330(40)	280(40)	-50(30)	40(30)	-70(30)
C(23B)	340(40)	440(40)	340(40)	50(40)	70(40)	-50(40)
C(24B)	370(50)	400(40)	430(40)	-80(40)	-80(40)	-120(40)
C(25B)	320(50)	420(40)	500(50)	70(40)	50(40)	-50(40)
C(26B)	220(40)	170(40)	190(40)	-30(30)	-30(30)	20(30)
C(27B)	230(40)	300(40)	310(40)	-30(30)	-90(30)	-40(30)
C(28B)	260(40)	300(40)	210(40)	-50(30)	20(30)	60(30)
C(29B)	190(40)	200(40)	210(40)	0(30)	-10(30)	-20(30)
C(30B)	200(40)	200(40)	130(40)	-30(30)	-40(30)	-30(30)
C(31B)	210(40)	260(40)	190(40)	80(30)	-30(30)	60(30)
C(32B)	310(40)	260(40)	240(40)	80(30)	-30(30)	-40(30)
C(33B)	240(40)	240(40)	270(40)	10(30)	10(30)	-20(30)
C(34B)	220(40)	180(40)	200(40)	-50(30)	-50(30)	40(30)
C(35B)	300(40)	240(40)	270(40)	-60(30)	10(30)	-20(30)
C(36B)	330(40)	240(40)	260(40)	-30(30)	-80(30)	50(30)
C(37B)	290(40)	350(40)	300(40)	-50(30)	-100(30)	-20(30)
C(38B)	210(40)	230(40)	240(40)	-50(30)	10(30)	-30(30)
C(39B)	240(40)	390(40)	270(40)	-40(30)	20(30)	-60(30)
C(40B)	160(40)	280(40)	200(40)	-20(30)	-70(30)	60(30)
C(41B)	260(40)	350(40)	250(40)	-20(30)	70(30)	30(30)
C(42B)	150(40)	250(40)	180(40)	-90(30)	10(30)	80(30)
C(43B)	240(40)	290(40)	230(40)	-20(30)	0(30)	30(30)
C(44B)	220(40)	380(40)	220(40)	-50(30)	-20(30)	30(30)

C(45B)	430(50)	440(50)	390(40)	-200(40)	80(40)	0(40)
C(46B)	180(40)	230(40)	240(40)	-60(30)	30(30)	50(30)
C(47B)	310(40)	350(40)	330(40)	-80(40)	0(40)	30(40)
C(48B)	290(40)	250(40)	260(40)	-40(30)	40(30)	-10(30)
C(49B)	330(40)	310(40)	340(40)	0(30)	100(40)	10(40)
C(50B)	220(40)	260(40)	180(40)	-30(30)	60(30)	60(30)
Ir(3)	203(2)	293(3)	115(2)	-46(2)	30(2)	16(2)
P(1C)	227(15)	370(16)	176(13)	-119(12)	20(11)	36(12)
P(2C)	227(14)	179(13)	176(13)	-20(11)	-62(11)	18(11)
O(1C)	220(30)	270(30)	150(30)	-40(20)	-10(30)	20(30)
O(2C)	210(30)	290(30)	180(30)	-10(30)	30(30)	10(30)
N(1C)	120(30)	200(30)	100(30)	-20(30)	30(30)	20(30)
C(1C)	280(40)	230(40)	140(40)	-30(30)	-20(30)	20(30)
C(2C)	340(40)	320(40)	270(40)	-100(30)	-40(40)	0(40)
C(3C)	390(50)	360(40)	390(40)	-170(40)	-20(40)	20(40)
C(4C)	490(50)	530(50)	540(50)	-170(40)	-110(40)	-70(40)
C(5C)	340(40)	350(40)	340(40)	-150(40)	-10(40)	-40(40)
C(6C)	240(40)	260(40)	200(40)	-50(30)	40(30)	-40(30)
C(7C)	140(40)	190(40)	120(30)	-50(30)	40(30)	0(30)
C(8C)	280(40)	360(40)	310(40)	-10(40)	20(30)	-100(40)
C(9C)	250(40)	300(40)	220(40)	-150(30)	30(30)	-30(30)
C(10C)	280(40)	250(40)	280(40)	-150(30)	0(30)	-30(30)
C(11C)	190(40)	190(40)	160(40)	-20(30)	-50(30)	0(30)
C(12C)	150(40)	170(40)	140(40)	-10(30)	-20(30)	-10(30)
C(13C)	180(40)	230(40)	190(40)	-30(30)	0(30)	40(30)
C(14C)	140(40)	180(40)	230(40)	-40(30)	-50(30)	90(30)
C(15C)	250(40)	300(40)	390(40)	-40(40)	-10(40)	-20(30)
C(16C)	120(40)	240(40)	240(40)	30(30)	40(30)	0(30)

C(17C)	210(40)	260(40)	240(40)	-30(30)	-10(30)	20(30)
C(18C)	410(50)	370(40)	330(40)	-120(40)	-70(40)	-50(40)
C(19C)	400(50)	400(40)	340(40)	-40(40)	-30(40)	100(40)
C(20C)	410(50)	380(40)	310(40)	-60(40)	-10(40)	50(40)
C(21C)	580(50)	450(50)	520(50)	-160(40)	-90(40)	30(40)
C(22C)	700(60)	790(60)	880(60)	-140(40)	-60(40)	-50(40)
C(23C)	2660(150)	2860(150)	2690(150)	-500(50)	-220(50)	-60(50)
C(24C)	3500(200)	3500(200)	3600(200)	-530(60)	-250(50)	-10(50)
C(25C)	560(50)	670(50)	680(50)	-130(40)	-10(40)	-110(40)
C(26C)	430(50)	510(50)	480(50)	-190(40)	120(40)	-70(40)
C(27C)	410(50)	600(50)	410(50)	-80(40)	10(40)	-20(40)
C(28C)	500(50)	770(50)	570(50)	-190(40)	-30(40)	50(40)
C(29C)	550(50)	590(50)	510(50)	-210(40)	80(40)	-50(40)
C(30C)	240(40)	280(40)	330(40)	-120(30)	-50(30)	40(30)
C(31C)	350(40)	420(40)	390(40)	-130(40)	-20(40)	20(40)
C(32C)	560(50)	520(50)	550(50)	-170(40)	-170(40)	80(40)
C(33C)	480(50)	460(50)	420(40)	-190(40)	-50(40)	-10(40)
C(34C)	250(40)	190(40)	290(40)	20(30)	10(30)	-10(30)
C(35C)	360(40)	370(40)	320(40)	0(40)	-10(40)	-40(40)
C(36C)	400(50)	410(40)	440(50)	80(40)	50(40)	-80(40)
C(37C)	320(40)	400(40)	300(40)	0(30)	70(40)	0(40)
C(38C)	210(40)	230(40)	160(40)	50(30)	-10(30)	100(30)
C(39C)	530(50)	520(50)	400(50)	0(40)	-40(40)	110(40)
C(40C)	250(40)	320(40)	230(40)	-30(30)	-70(30)	10(30)
C(41C)	310(40)	390(40)	280(40)	-30(30)	0(40)	90(40)
C(42C)	310(40)	370(40)	240(40)	-60(30)	-30(40)	50(40)
C(43C)	690(50)	670(50)	570(50)	-180(40)	-160(40)	30(40)
C(44C)	240(40)	290(40)	340(40)	-20(30)	-10(30)	-20(30)
C(45C)	320(40)	330(40)	450(40)	-70(40)	-50(40)	-30(30)

C(46C)	190(40)	210(40)	260(40)	-40(30)	-30(30)	20(30)
C(47C)	350(40)	300(40)	260(40)	30(30)	50(40)	-30(40)
C(48C)	270(40)	330(40)	250(40)	-50(30)	0(30)	20(30)
C(49C)	300(40)	370(40)	370(40)	-100(30)	-40(40)	80(40)
C(50C)	200(40)	270(40)	160(40)	-10(30)	40(30)	20(30)
Ir(4)	247(2)	376(3)	113(2)	-24(2)	63(2)	60(2)
P(1D)	368(16)	342(15)	118(12)	-44(12)	-26(11)	40(14)
P(2D)	192(14)	311(15)	234(14)	-20(12)	22(11)	64(12)
O(1D)	230(30)	310(30)	190(30)	10(30)	20(30)	30(30)
O(2D)	290(30)	340(30)	200(30)	10(30)	110(30)	50(30)
N(1D)	180(30)	150(30)	120(30)	0(30)	30(30)	-10(30)
C(1D)	290(40)	320(40)	190(40)	-30(30)	0(30)	50(40)
C(2D)	320(40)	310(40)	180(40)	10(30)	-40(30)	30(40)
C(3D)	350(40)	340(40)	260(40)	-30(30)	-120(40)	100(40)
C(4D)	260(40)	310(40)	260(40)	-100(30)	-60(30)	80(30)
C(5D)	210(40)	310(40)	210(40)	-50(30)	10(30)	40(30)
C(6D)	260(40)	220(40)	160(40)	-40(30)	-20(30)	10(30)
C(7D)	170(40)	280(40)	170(40)	10(30)	-50(30)	50(30)
C(8D)	140(40)	260(40)	170(40)	-10(30)	-20(30)	70(30)
C(9D)	240(40)	350(40)	240(40)	-100(30)	50(30)	-30(30)
C(10D)	190(40)	200(40)	160(40)	30(30)	20(30)	0(30)
C(11D)	160(40)	210(40)	130(40)	-30(30)	-20(30)	0(30)
C(12D)	150(40)	240(40)	120(40)	-50(30)	-30(30)	-40(30)
C(13D)	210(40)	230(40)	180(40)	-50(30)	-20(30)	20(30)
C(14D)	240(40)	240(40)	220(40)	-40(30)	-50(30)	-90(30)
C(15D)	210(40)	260(40)	270(40)	-80(30)	50(30)	50(30)
C(16D)	290(40)	290(40)	250(40)	-50(30)	-10(30)	90(30)
C(17D)	200(40)	330(40)	240(40)	-50(30)	-50(30)	20(30)

C(18D)	370(40)	320(40)	320(40)	-70(40)	10(40)	40(40)
C(19D)	500(50)	490(50)	400(50)	-60(40)	50(40)	-50(40)
C(20D)	330(40)	310(40)	260(40)	10(30)	-30(40)	20(40)
C(21D)	510(50)	440(50)	430(50)	70(40)	-60(40)	30(40)
C(22D)	450(50)	450(50)	450(50)	-90(40)	-60(40)	40(40)
C(23D)	580(50)	610(50)	520(50)	-120(40)	-140(40)	230(40)
C(24D)	240(40)	240(40)	240(40)	60(30)	20(30)	20(30)
C(25D)	650(50)	710(50)	800(50)	-140(40)	-190(40)	80(40)
C(26D)	290(40)	390(40)	320(40)	-40(40)	50(40)	20(40)
C(27D)	440(50)	730(50)	510(50)	10(40)	30(40)	70(40)
C(28D)	480(50)	500(50)	380(40)	-70(40)	30(40)	50(40)
C(29D)	460(50)	460(50)	380(40)	20(40)	140(40)	70(40)
C(30D)	240(40)	200(40)	270(40)	-10(30)	-50(30)	-10(30)
C(31D)	570(50)	620(50)	550(50)	0(40)	-110(40)	-100(40)
C(32D)	770(60)	910(60)	750(60)	150(40)	-130(40)	-120(40)
C(33D)	890(60)	860(60)	740(60)	-120(40)	-70(40)	130(40)
C(34D)	430(50)	350(40)	350(40)	-70(40)	130(40)	90(40)
C(35D)	520(50)	460(50)	380(40)	-220(40)	30(40)	-10(40)
C(36D)	480(50)	520(50)	440(50)	-140(40)	70(40)	60(40)
C(37D)	600(50)	510(50)	480(50)	-100(40)	40(40)	90(40)
C(38D)	450(50)	380(40)	250(40)	-80(30)	0(40)	110(40)
C(39D)	650(50)	560(50)	520(50)	-210(40)	-60(40)	40(40)
C(40D)	390(50)	340(40)	310(40)	-30(30)	-10(40)	30(40)
C(41D)	500(50)	500(50)	520(50)	-20(40)	-90(40)	-50(40)
C(42D)	380(40)	360(40)	280(40)	-40(40)	-30(40)	10(40)
C(43D)	440(50)	430(50)	400(40)	-30(40)	0(40)	-20(40)
C(44D)	500(50)	500(50)	480(50)	-40(40)	-60(40)	0(40)
C(45D)	620(50)	570(50)	660(50)	-80(40)	-160(40)	70(40)
C(46D)	180(40)	340(40)	200(40)	50(30)	-70(30)	50(30)

C(47D)	330(40)	370(40)	250(40)	-60(30)	-20(40)	-50(40)
C(48D)	290(40)	450(40)	380(40)	0(40)	50(40)	0(40)
C(49D)	420(50)	430(50)	530(50)	-120(40)	0(40)	40(40)
C(50D)	250(40)	330(40)	400(40)	-70(40)	140(40)	0(30)
C(1E)	370(50)	420(50)	420(50)	-80(40)	-70(40)	60(40)
C(2E)	330(50)	340(40)	490(50)	50(40)	-40(40)	20(40)
C(3E)	300(40)	440(50)	250(40)	120(40)	-70(40)	20(40)
C(1F)	380(50)	520(50)	390(50)	-160(40)	-20(40)	0(40)
C(2F)	340(50)	410(40)	510(50)	-130(40)	-60(40)	-30(40)
C(3F)	420(50)	520(50)	490(50)	-120(40)	-100(40)	-80(40)
P(2)	255(16)	414(17)	271(15)	-147(13)	-16(13)	19(13)
F(1B)	530(30)	670(30)	190(30)	0(30)	70(30)	200(30)
F(2B)	410(30)	750(40)	450(30)	-100(30)	60(30)	-90(30)
F(3B)	360(30)	500(30)	300(30)	-110(20)	-120(20)	30(30)
F(4B)	420(30)	440(30)	420(30)	-130(30)	90(30)	30(30)
F(5B)	610(40)	770(40)	770(40)	-240(30)	-490(30)	-20(30)
F(6B)	570(40)	510(30)	540(30)	-260(30)	-40(30)	180(30)
P(3)	212(15)	409(17)	233(14)	-36(13)	28(12)	-13(13)
F(1C)	470(30)	610(30)	420(30)	-190(30)	110(30)	160(30)
F(2C)	500(30)	430(30)	390(30)	-240(30)	100(30)	-150(30)
F(3C)	370(30)	920(40)	530(30)	-80(30)	-120(30)	80(30)
F(4C)	460(30)	490(30)	490(30)	40(30)	-40(30)	-100(30)
F(5C)	670(40)	570(30)	620(40)	-70(30)	100(30)	-200(30)
F(6C)	170(30)	680(30)	180(30)	90(20)	-20(20)	90(20)

(ONO^{tBu})Ir(PPh$_3$)$_2$Ph, 17

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The two benzene molecules of salvation were restrained to regular hexagons with isotropic displacement parameters restrained and refined to one overall value. Because of the symmetry in the overall structure (2-fold around the *b*-axis) the occupancies of the benzene needs to be refined as packing is impossible otherwise.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S58. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **17**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ir(1)	10000	1839(1)	7500	16(1)	1
P(1)	8517(1)	1863(1)	7579(1)	18(1)	1
O(1)	9730(1)	1839(1)	6624(1)	19(1)	1
N(1)	10000	815(1)	7500	15(1)	1
C(1)	10077(1)	1406(1)	6272(1)	18(1)	1
C(2)	10099(2)	1539(1)	5660(1)	20(1)	1
C(3)	10612(2)	1158(1)	5320(1)	22(1)	1
C(4)	11085(1)	630(1)	5524(1)	20(1)	1
C(5)	10946(1)	450(1)	6091(1)	20(1)	1
C(6)	10421(1)	811(1)	6463(1)	17(1)	1
C(7)	10194(1)	475(1)	7011(1)	16(1)	1
C(8)	10153(1)	-197(1)	7002(1)	19(1)	1
C(9)	10000	-575(2)	7500	24(1)	1

C(10)	9549(2)	2066(1)	5384(1)	24(1)	1
C(11)	9759(2)	2751(1)	5602(1)	29(1)	1
C(12)	8639(2)	1901(1)	5526(1)	27(1)	1
C(13)	9628(2)	2074(1)	4723(1)	31(1)	1
C(14)	11703(2)	282(1)	5130(1)	24(1)	1
C(15)	12440(2)	733(1)	5010(1)	36(1)	1
C(16)	11281(2)	92(1)	4554(1)	35(1)	1
C(17)	12045(2)	-341(1)	5409(1)	31(1)	1
C(18)	10000	-1297(1)	7500	24(1)	1
C(19)	10095(3)	-1586(2)	6854(2)	25(1)	0.50
C(20)	10662(4)	-1542(2)	7856(2)	32(1)	0.50
C(21)	9120(4)	-1536(2)	7684(2)	32(1)	0.50
C(22)	7954(2)	2271(1)	6989(1)	22(1)	1
C(23)	8230(2)	2861(1)	6767(1)	24(1)	1
C(24)	7754(2)	3197(1)	6357(1)	28(1)	1
C(25)	7020(2)	2936(1)	6160(1)	34(1)	1
C(26)	6743(2)	2344(1)	6367(1)	38(1)	1
C(27)	7204(2)	2014(1)	6785(1)	30(1)	1
C(28)	8029(1)	1058(1)	7562(1)	20(1)	1
C(29)	8215(1)	659(1)	7088(1)	22(1)	1
C(30)	7867(2)	44(1)	7041(1)	28(1)	1
C(31)	7326(2)	-185(1)	7457(1)	31(1)	1
C(32)	7132(2)	210(1)	7925(1)	34(1)	1
C(33)	7481(2)	825(1)	7978(1)	27(1)	1
C(34)	8067(1)	2292(1)	8205(1)	22(1)	1
C(35)	7742(2)	2916(1)	8141(1)	30(1)	1
C(36)	7501(2)	3281(1)	8617(1)	36(1)	1
C(37)	7579(2)	3018(1)	9169(1)	32(1)	1
C(38)	7881(2)	2399(1)	9236(1)	28(1)	1

C(39)	8134(2)	2032(1)	8762(1)	23(1)	1
C(40)	10000	2850(1)	7500	16(1)	1
C(41)	10317(2)	3210(1)	7036(1)	24(1)	1
C(42)	10309(2)	3890(1)	7037(1)	33(1)	1
C(43)	10000	4233(1)	7500	24(1)	1
C(51)	5298(6)	-143(3)	5791(4)	173(2)	0.440(4)
C(52)	5967(5)	96(4)	6107(3)	173(2)	0.440(4)
C(53)	6385(4)	650(4)	5921(3)	173(2)	0.440(4)
C(54)	6134(5)	965(4)	5419(3)	173(2)	0.440(4)
C(55)	5466(6)	726(5)	5103(2)	173(2)	0.440(4)
C(56)	5047(5)	172(4)	5289(3)	173(2)	0.440(4)
C(61)	4279(5)	1643(4)	6575(3)	173(2)	0.560(4)
C(62)	4791(5)	1396(4)	7006(3)	173(2)	0.560(4)
C(63)	5312(5)	872(4)	6890(2)	173(2)	0.560(4)
C(64)	5321(4)	594(3)	6343(2)	173(2)	0.560(4)
C(65)	4809(3)	841(3)	5912(2)	173(2)	0.560(4)
C(66)	4288(4)	1365(4)	6028(3)	173(2)	0.560(4)

Table S59. Selected bond lengths [Å] and angles [°] for **17**.

Ir(1)-O(1)	2.0744(12)	O(1)-Ir(1)-C(40)	90.05(4)
Ir(1)-C(40)	2.074(3)	O(1)-Ir(1)-O(1)#1	179.91(8)
Ir(1)-O(1)#1	2.0744(12)	C(40)-Ir(1)-O(1)#1	90.04(4)
Ir(1)-N(1)	2.103(2)	O(1)-Ir(1)-N(1)	89.95(4)
Ir(1)-P(1)#1	2.3921(6)	C(40)-Ir(1)-N(1)	180.0
Ir(1)-P(1)	2.3921(6)	O(1)#1-Ir(1)-N(1)	89.96(4)
		O(1)-Ir(1)-P(1)#1	97.70(4)
		C(40)-Ir(1)-P(1)#1	88.831(13)
		O(1)#1-Ir(1)-P(1)#1	82.30(4)
		N(1)-Ir(1)-P(1)#1	91.169(13)
		O(1)-Ir(1)-P(1)	82.30(4)
		C(40)-Ir(1)-P(1)	88.829(13)
		O(1)#1-Ir(1)-P(1)	97.70(4)
		N(1)-Ir(1)-P(1)	91.171(13)
		P(1)#1-Ir(1)-P(1)	177.66(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2

Table S60. Bond lengths [Å] and angles [°] for **17**.

Ir(1)-O(1)	2.0744(12)	P(1)-C(22)	1.841(2)
Ir(1)-C(40)	2.074(3)	P(1)-C(34)	1.844(2)
Ir(1)-O(1)#1	2.0744(12)	O(1)-C(1)	1.329(2)
Ir(1)-N(1)	2.103(2)	N(1)-C(7)	1.367(2)
Ir(1)-P(1)#1	2.3921(6)	N(1)-C(7)#1	1.367(2)
Ir(1)-P(1)	2.3921(6)	C(1)-C(6)	1.412(3)
P(1)-C(28)	1.830(2)	C(1)-C(2)	1.446(2)

C(2)-C(3)	1.382(3)	C(28)-C(33)	1.391(3)
C(2)-C(10)	1.537(3)	C(28)-C(29)	1.401(3)
C(3)-C(4)	1.407(3)	C(29)-C(30)	1.385(3)
C(4)-C(5)	1.383(2)	C(30)-C(31)	1.381(3)
C(4)-C(14)	1.526(3)	C(31)-C(32)	1.390(3)
C(5)-C(6)	1.415(3)	C(32)-C(33)	1.388(3)
C(6)-C(7)	1.490(3)	C(34)-C(35)	1.390(3)
C(7)-C(8)	1.381(3)	C(34)-C(39)	1.401(3)
C(8)-C(9)	1.412(3)	C(35)-C(36)	1.389(3)
C(9)-C(8)#1	1.412(3)	C(36)-C(37)	1.393(3)
C(9)-C(18)	1.483(4)	C(37)-C(38)	1.370(3)
C(10)-C(11)	1.531(3)	C(38)-C(39)	1.393(3)
C(10)-C(12)	1.538(3)	C(40)-C(41)#1	1.400(3)
C(10)-C(13)	1.538(3)	C(40)-C(41)	1.400(3)
C(14)-C(15)	1.529(3)	C(41)-C(42)	1.395(3)
C(14)-C(17)	1.535(3)	C(42)-C(43)	1.376(3)
C(14)-C(16)	1.547(3)	C(43)-C(42)#1	1.376(3)
C(18)-C(20)#1	1.437(5)	C(51)-C(52)	1.3900
C(18)-C(20)	1.437(5)	C(51)-C(56)	1.3900
C(18)-C(21)	1.557(5)	C(52)-C(53)	1.3900
C(18)-C(21)#1	1.557(5)	C(53)-C(54)	1.3900
C(18)-C(19)	1.617(4)	C(54)-C(55)	1.3900
C(18)-C(19)#1	1.617(4)	C(55)-C(56)	1.3900
C(22)-C(23)	1.389(3)	C(61)-C(62)	1.3900
C(22)-C(27)	1.398(3)	C(61)-C(66)	1.3900
C(23)-C(24)	1.401(3)	C(62)-C(63)	1.3900
C(24)-C(25)	1.374(4)	C(63)-C(64)	1.3900
C(25)-C(26)	1.380(4)	C(64)-C(65)	1.3900
C(26)-C(27)	1.395(3)	C(65)-C(66)	1.3900

		C(3)-C(2)-C(1)	117.89(19)
O(1)-Ir(1)-C(40)	90.05(4)	C(3)-C(2)-C(10)	120.30(16)
O(1)-Ir(1)-O(1)#1	179.91(8)	C(1)-C(2)-C(10)	121.76(18)
C(40)-Ir(1)-O(1)#1	90.04(4)	C(2)-C(3)-C(4)	124.52(17)
O(1)-Ir(1)-N(1)	89.95(4)	C(5)-C(4)-C(3)	115.93(19)
C(40)-Ir(1)-N(1)	180.0	C(5)-C(4)-C(14)	123.29(19)
O(1)#1-Ir(1)-N(1)	89.96(4)	C(3)-C(4)-C(14)	120.78(16)
O(1)-Ir(1)-P(1)#1	97.70(4)	C(4)-C(5)-C(6)	122.38(19)
C(40)-Ir(1)-P(1)#1	88.831(13)	C(1)-C(6)-C(5)	119.76(16)
O(1)#1-Ir(1)-P(1)#1	82.30(4)	C(1)-C(6)-C(7)	124.81(18)
N(1)-Ir(1)-P(1)#1	91.169(13)	C(5)-C(6)-C(7)	114.99(18)
O(1)-Ir(1)-P(1)	82.30(4)	N(1)-C(7)-C(8)	120.79(17)
C(40)-Ir(1)-P(1)	88.829(13)	N(1)-C(7)-C(6)	121.71(18)
O(1)#1-Ir(1)-P(1)	97.70(4)	C(8)-C(7)-C(6)	117.44(16)
N(1)-Ir(1)-P(1)	91.171(13)	C(7)-C(8)-C(9)	122.98(19)
P(1)#1-Ir(1)-P(1)	177.66(3)	C(8)-C(9)-C(8)#1	113.4(3)
C(28)-P(1)-C(22)	100.60(10)	C(8)-C(9)-C(18)	123.31(14)
C(28)-P(1)-C(34)	106.30(10)	C(8)#1-C(9)-C(18)	123.31(14)
C(22)-P(1)-C(34)	100.04(10)	C(11)-C(10)-C(2)	112.48(18)
C(28)-P(1)-Ir(1)	114.02(7)	C(11)-C(10)-C(12)	110.00(19)
C(22)-P(1)-Ir(1)	116.26(8)	C(2)-C(10)-C(12)	107.67(18)
C(34)-P(1)-Ir(1)	117.41(8)	C(11)-C(10)-C(13)	107.52(19)
C(1)-O(1)-Ir(1)	120.86(12)	C(2)-C(10)-C(13)	111.93(18)
C(7)-N(1)-C(7)#1	118.5(2)	C(12)-C(10)-C(13)	107.10(19)
C(7)-N(1)-Ir(1)	120.73(11)	C(4)-C(14)-C(15)	109.24(18)
C(7)#1-N(1)-Ir(1)	120.73(11)	C(4)-C(14)-C(17)	111.80(16)
O(1)-C(1)-C(6)	123.46(15)	C(15)-C(14)-C(17)	107.7(2)
O(1)-C(1)-C(2)	119.12(18)	C(4)-C(14)-C(16)	110.4(2)
C(6)-C(1)-C(2)	117.41(17)	C(15)-C(14)-C(16)	109.62(18)

C(17)-C(14)-C(16)	108.05(18)	C(26)-C(27)-C(22)	120.6(2)
C(20)#1-C(18)-C(20)	139.1(5)	C(33)-C(28)-C(29)	118.5(2)
C(20)#1-C(18)-C(9)	110.5(2)	C(33)-C(28)-P(1)	124.55(16)
C(20)-C(18)-C(9)	110.5(2)	C(29)-C(28)-P(1)	116.97(16)
C(20)#1-C(18)-C(21)	51.2(3)	C(30)-C(29)-C(28)	120.6(2)
C(20)-C(18)-C(21)	114.0(3)	C(31)-C(30)-C(29)	120.6(2)
C(9)-C(18)-C(21)	108.4(2)	C(30)-C(31)-C(32)	119.2(2)
C(20)#1-C(18)-C(21)#1	114.0(3)	C(33)-C(32)-C(31)	120.5(2)
C(20)-C(18)-C(21)#1	51.2(3)	C(32)-C(33)-C(28)	120.6(2)
C(9)-C(18)-C(21)#1	108.4(2)	C(35)-C(34)-C(39)	118.51(19)
C(21)-C(18)-C(21)#1	143.3(4)	C(35)-C(34)-P(1)	120.26(15)
C(20)#1-C(18)-C(19)	53.9(3)	C(39)-C(34)-P(1)	120.82(16)
C(20)-C(18)-C(19)	109.4(3)	C(36)-C(35)-C(34)	121.2(2)
C(9)-C(18)-C(19)	111.50(18)	C(35)-C(36)-C(37)	119.6(2)
C(21)-C(18)-C(19)	103.0(3)	C(38)-C(37)-C(36)	119.7(2)
C(21)#1-C(18)-C(19)	62.9(3)	C(37)-C(38)-C(39)	121.0(2)
C(20)#1-C(18)-C(19)#1	109.4(3)	C(38)-C(39)-C(34)	119.9(2)
C(20)-C(18)-C(19)#1	54.0(3)	C(41)#1-C(40)-C(41)	116.2(3)
C(9)-C(18)-C(19)#1	111.50(18)	C(41)#1-C(40)-Ir(1)	121.88(13)
C(21)-C(18)-C(19)#1	62.9(3)	C(41)-C(40)-Ir(1)	121.88(13)
C(21)#1-C(18)-C(19)#1	103.0(3)	C(42)-C(41)-C(40)	121.6(2)
C(19)-C(18)-C(19)#1	137.0(4)	C(43)-C(42)-C(41)	121.2(2)
C(23)-C(22)-C(27)	118.6(2)	C(42)-C(43)-C(42)#1	118.3(3)
C(23)-C(22)-P(1)	120.99(18)	C(52)-C(51)-C(56)	120.0
C(27)-C(22)-P(1)	120.23(17)	C(53)-C(52)-C(51)	120.0
C(22)-C(23)-C(24)	120.5(2)	C(52)-C(53)-C(54)	120.0
C(25)-C(24)-C(23)	120.1(2)	C(55)-C(54)-C(53)	120.0
C(24)-C(25)-C(26)	120.3(2)	C(54)-C(55)-C(56)	120.0
C(25)-C(26)-C(27)	119.9(3)	C(55)-C(56)-C(51)	120.0

C(62)-C(61)-C(66)	120.0
C(63)-C(62)-C(61)	120.0
C(62)-C(63)-C(64)	120.0
C(63)-C(64)-C(65)	120.0
C(66)-C(65)-C(64)	120.0
C(65)-C(66)-C(61)	120.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2

Table S61. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **17**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	221(1)	123(1)	128(1)	0	2(1)	0
P(1)	202(2)	144(2)	180(2)	4(2)	13(2)	19(2)
O(1)	258(8)	184(7)	137(5)	-3(5)	-2(5)	28(6)
N(1)	174(10)	131(9)	143(8)	0	-18(11)	0
C(1)	213(12)	168(8)	142(6)	-6(6)	-12(8)	-3(9)
C(2)	271(14)	185(9)	142(7)	6(6)	-18(8)	8(9)
C(3)	296(13)	224(11)	133(8)	5(7)	15(8)	24(9)
C(4)	269(12)	188(10)	154(8)	-19(7)	20(8)	9(9)
C(5)	264(12)	154(9)	170(8)	-2(7)	-1(8)	0(8)
C(6)	206(11)	182(9)	132(7)	-13(7)	-4(7)	-7(8)
C(7)	192(11)	161(9)	137(7)	-6(7)	-6(6)	0(7)
C(8)	231(14)	160(9)	185(8)	-19(7)	34(7)	-5(7)
C(9)	167(13)	275(14)	289(12)	0	16(15)	0
C(10)	313(13)	253(11)	147(8)	25(8)	-19(8)	63(10)
C(11)	391(15)	224(11)	263(10)	43(9)	-12(9)	55(10)
C(12)	301(13)	309(13)	195(8)	-28(8)	-48(8)	60(10)
C(13)	421(15)	358(14)	164(9)	41(9)	7(9)	108(12)
C(14)	331(14)	208(11)	167(8)	11(7)	50(8)	56(9)
C(15)	384(16)	285(13)	400(12)	36(10)	136(11)	68(12)
C(16)	490(18)	376(15)	191(9)	-65(9)	21(10)	126(13)
C(17)	456(17)	255(12)	222(9)	14(8)	81(10)	106(11)

C(18)	289(15)	122(11)	317(13)	0	108(17)	0
C(19)	340(30)	141(17)	265(17)	-49(14)	77(19)	-30(19)
C(20)	420(30)	200(20)	330(20)	-6(18)	-80(20)	60(20)
C(21)	390(30)	200(20)	380(20)	-1(19)	140(20)	-70(20)
C(22)	267(13)	182(10)	202(9)	17(8)	-3(8)	58(9)
C(23)	261(13)	238(11)	212(9)	-2(8)	22(8)	45(9)
C(24)	301(14)	287(12)	263(10)	75(9)	26(9)	47(11)
C(25)	277(14)	391(15)	349(12)	140(11)	-35(10)	47(11)
C(26)	261(14)	421(16)	457(14)	125(12)	-99(11)	6(12)
C(27)	274(14)	272(12)	360(11)	96(9)	-4(10)	29(10)
C(28)	207(10)	183(9)	211(9)	2(7)	-44(8)	8(7)
C(29)	228(12)	211(11)	216(9)	-22(7)	-20(8)	15(9)
C(30)	319(14)	237(12)	298(11)	-55(9)	-44(10)	19(10)
C(31)	374(13)	210(10)	360(12)	-4(10)	-61(12)	-62(9)
C(32)	398(16)	304(13)	304(11)	34(10)	24(10)	-98(12)
C(33)	325(14)	255(12)	228(9)	-14(8)	35(9)	-62(11)
C(34)	229(12)	198(10)	219(9)	-11(8)	64(8)	16(9)
C(35)	417(16)	216(11)	264(10)	29(9)	103(10)	55(11)
C(36)	487(19)	227(12)	365(12)	-11(9)	154(12)	72(12)
C(37)	389(16)	284(12)	277(10)	-59(9)	139(10)	22(11)
C(38)	352(15)	276(12)	203(9)	-11(8)	76(9)	23(10)
C(39)	265(12)	193(10)	219(9)	-8(8)	40(8)	15(9)
C(40)	157(12)	149(11)	165(9)	0	-51(13)	0
C(41)	246(11)	208(11)	261(9)	40(9)	-7(8)	0(10)
C(42)	340(14)	221(12)	437(13)	108(10)	-6(11)	-46(11)
C(43)	270(9)	97(7)	339(9)	0	5(9)	0

(ONO^{tBu})Ir(PPh$_3$)[κ^2-(*o*-C$_6$H$_4$)PPh$_2$], 18

Crystals were mounted on a glass fiber using Paratone oil, then placed on the diffractometer under a nitrogen stream at 100K.

The solvent region is disordered and we were unable to establish any solvent model so the contribution of the solvent region to the observed intensities was removed with SQUEEZE[2]. Two solvent voids of 1920Å^3 each were assigned 291 electrons each. This is a reasonable approximation of eight *n*-butyl ether solvents.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S62. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **18**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ir(1)	6253(1)	4201(1)	1358(1)	12(1)	1
P(1)	6026(1)	3528(1)	333(1)	15(1)	1
P(2)	6318(1)	4857(1)	2366(1)	14(1)	1
O(1)	6403(1)	3395(1)	2082(1)	15(1)	1
O(2)	6132(1)	5067(1)	693(1)	14(1)	1
N(1)	6763(1)	4218(1)	1351(1)	13(1)	1
C(1)	6595(1)	2868(1)	2016(1)	14(1)	1
C(2)	6581(1)	2208(1)	2339(1)	16(1)	1
C(3)	6738(1)	1627(1)	2177(1)	19(1)	1
C(4)	6916(1)	1648(1)	1714(1)	19(1)	1
C(5)	6956(1)	2300(1)	1472(1)	18(1)	1
C(6)	6819(1)	2924(1)	1638(1)	15(1)	1
C(7)	6952(1)	3607(1)	1476(1)	14(1)	1

C(8)	7288(1)	3612(1)	1472(1)	17(1)	1
C(9)	7425(1)	4204(1)	1268(1)	17(1)	1
C(10)	7222(1)	4800(1)	1128(1)	16(1)	1
C(11)	6902(1)	4823(1)	1211(1)	14(1)	1
C(12)	6720(1)	5515(1)	1111(1)	14(1)	1
C(13)	6936(1)	6116(1)	1254(1)	17(1)	1
C(14)	6813(1)	6788(1)	1052(1)	19(1)	1
C(15)	6452(1)	6849(1)	696(1)	19(1)	1
C(16)	6222(1)	6291(1)	562(1)	16(1)	1
C(17)	6356(1)	5595(1)	803(1)	14(1)	1
C(18)	6386(1)	2146(1)	2851(1)	21(1)	1
C(19)	5994(1)	2301(2)	2482(1)	33(1)	1
C(20)	6419(1)	1398(1)	3170(1)	36(1)	1
C(21)	6546(1)	2674(1)	3451(1)	31(1)	1
C(22)	7052(1)	979(1)	1483(1)	24(1)	1
C(23)	6787(1)	745(2)	775(1)	37(1)	1
C(24)	7112(1)	367(1)	1997(1)	45(1)	1
C(25)	7400(1)	1134(1)	1410(1)	34(1)	1
C(26)	7772(1)	4183(1)	1167(1)	22(1)	1
C(27)	7699(1)	3860(2)	447(1)	46(1)	1
C(28)	7929(1)	4912(2)	1182(2)	43(1)	1
C(29)	8036(1)	3720(2)	1719(1)	37(1)	1
C(30)	7056(1)	7432(1)	1155(1)	26(1)	1
C(31A)	7196(5)	7474(8)	630(7)	83(7)	0.420(12)
C(32A)	6863(4)	8112(7)	1249(9)	89(6)	0.420(12)
C(33A)	7345(2)	7402(5)	1898(4)	39(2)	0.420(12)
C(31B)	7450(2)	7244(4)	1519(6)	69(4)	0.580(12)
C(32B)	7018(3)	7726(5)	417(4)	51(3)	0.580(12)
C(33B)	6974(4)	8015(6)	1528(7)	111(7)	0.580(12)

C(34)	5834(1)	6403(1)	111(1)	20(1)	1
C(35)	5743(1)	7181(1)	-80(1)	30(1)	1
C(36)	5759(1)	5997(1)	-574(1)	23(1)	1
C(37)	5594(1)	6158(1)	490(1)	25(1)	1
C(38)	5682(1)	3979(1)	-373(1)	16(1)	1
C(39)	5445(1)	4408(1)	-228(1)	19(1)	1
C(40)	5157(1)	4669(1)	-761(1)	22(1)	1
C(41)	5103(1)	4517(1)	-1453(1)	24(1)	1
C(42)	5343(1)	4103(1)	-1601(1)	26(1)	1
C(43)	5630(1)	3829(1)	-1071(1)	21(1)	1
C(44)	5810(1)	2685(1)	338(1)	19(1)	1
C(45)	5998(1)	2104(1)	708(1)	25(1)	1
C(46)	5836(1)	1462(1)	724(1)	34(1)	1
C(47)	5481(1)	1394(2)	378(1)	42(1)	1
C(48)	5287(1)	1963(2)	13(1)	42(1)	1
C(49)	5452(1)	2602(1)	-11(1)	29(1)	1
C(50)	6337(1)	3333(1)	-82(1)	17(1)	1
C(51)	6408(1)	2657(1)	-251(1)	30(1)	1
C(52)	6650(1)	2558(2)	-559(1)	42(1)	1
C(53)	6825(1)	3138(2)	-695(1)	37(1)	1
C(54)	6753(1)	3810(1)	-539(1)	26(1)	1
C(55)	6510(1)	3909(1)	-235(1)	20(1)	1
C(56)	6283(1)	5812(1)	2418(1)	21(1)	1
C(57)	5972(1)	6130(2)	2366(1)	35(1)	1
C(58)	5948(1)	6864(2)	2391(1)	50(1)	1
C(59)	6231(1)	7278(2)	2471(1)	50(1)	1
C(60)	6541(1)	6962(2)	2521(1)	44(1)	1
C(61)	6570(1)	6237(1)	2500(1)	30(1)	1
C(62)	6655(1)	4600(1)	3190(1)	16(1)	1

C(63)	6582(1)	4507(1)	3791(1)	23(1)	1
C(64)	6840(1)	4274(1)	4404(1)	26(1)	1
C(65)	7174(1)	4142(1)	4421(1)	24(1)	1
C(66)	7249(1)	4243(1)	3830(1)	23(1)	1
C(67)	6988(1)	4462(1)	3214(1)	20(1)	1
C(68)	5907(1)	4477(1)	2271(1)	16(1)	1
C(69)	5713(1)	4422(1)	2691(1)	22(1)	1
C(70)	5415(1)	4014(1)	2455(1)	26(1)	1
C(71)	5306(1)	3704(1)	1801(1)	24(1)	1
C(72)	5499(1)	3775(1)	1377(1)	19(1)	1
C(73)	5812(1)	4150(1)	1608(1)	15(1)	1

Table S63. Selected bond lengths [Å] and angles [°] for **18**.

Ir(1)-O(1)	2.0602(14)	O(1)-Ir(1)-O(2)	175.07(6)
Ir(1)-O(2)	2.0719(14)	O(1)-Ir(1)-C(73)	80.87(7)
Ir(1)-C(73)	2.074(2)	O(2)-Ir(1)-C(73)	100.54(7)
Ir(1)-N(1)	2.1141(17)	O(1)-Ir(1)-N(1)	89.03(6)
Ir(1)-P(1)	2.3429(5)	O(2)-Ir(1)-N(1)	88.85(6)
Ir(1)-P(2)	2.3476(5)	C(73)-Ir(1)-N(1)	166.84(6)
		O(1)-Ir(1)-P(1)	99.46(4)
		O(2)-Ir(1)-P(1)	85.13(4)
		C(73)-Ir(1)-P(1)	95.93(6)
		N(1)-Ir(1)-P(1)	94.03(4)
		O(1)-Ir(1)-P(2)	81.03(4)
		O(2)-Ir(1)-P(2)	95.07(4)
		C(73)-Ir(1)-P(2)	68.10(6)
		N(1)-Ir(1)-P(2)	102.13(4)
		P(1)-Ir(1)-P(2)	163.84(2)

Table S64. Bond lengths [Å] and angles [°] for **18**.

Ir(1)-O(1)	2.0602(14)	P(1)-C(38)	1.826(2)
Ir(1)-O(2)	2.0719(14)	P(2)-C(68)	1.786(2)
Ir(1)-C(73)	2.074(2)	P(2)-C(62)	1.819(2)
Ir(1)-N(1)	2.1141(17)	P(2)-C(56)	1.816(3)
Ir(1)-P(1)	2.3429(5)	O(1)-C(1)	1.312(2)
Ir(1)-P(2)	2.3476(5)	O(2)-C(17)	1.321(2)
P(1)-C(50)	1.828(2)	N(1)-C(11)	1.357(3)
P(1)-C(44)	1.828(2)	N(1)-C(7)	1.365(3)

C(1)-C(6)	1.417(3)	C(26)-C(28)	1.519(4)
C(1)-C(2)	1.425(3)	C(26)-C(27)	1.528(3)
C(2)-C(3)	1.378(3)	C(26)-C(29)	1.528(3)
C(2)-C(18)	1.552(3)	C(30)-C(31A)	1.404(12)
C(3)-C(4)	1.407(3)	C(30)-C(33B)	1.454(9)
C(4)-C(5)	1.361(3)	C(30)-C(32A)	1.563(13)
C(4)-C(22)	1.529(3)	C(30)-C(31B)	1.561(7)
C(5)-C(6)	1.403(3)	C(30)-C(33A)	1.556(8)
C(6)-C(7)	1.487(3)	C(30)-C(32B)	1.571(8)
C(7)-C(8)	1.393(3)	C(34)-C(37)	1.544(3)
C(8)-C(9)	1.387(3)	C(34)-C(35)	1.531(3)
C(9)-C(10)	1.369(3)	C(34)-C(36)	1.536(3)
C(9)-C(26)	1.525(3)	C(38)-C(39)	1.387(3)
C(10)-C(11)	1.397(3)	C(38)-C(43)	1.402(3)
C(11)-C(12)	1.485(3)	C(39)-C(40)	1.378(3)
C(12)-C(13)	1.406(3)	C(40)-C(41)	1.391(3)
C(12)-C(17)	1.409(3)	C(41)-C(42)	1.382(3)
C(13)-C(14)	1.373(3)	C(42)-C(43)	1.380(3)
C(14)-C(15)	1.403(3)	C(44)-C(49)	1.394(3)
C(14)-C(30)	1.542(3)	C(44)-C(45)	1.397(3)
C(15)-C(16)	1.379(3)	C(45)-C(46)	1.390(3)
C(16)-C(17)	1.442(3)	C(46)-C(47)	1.382(4)
C(16)-C(34)	1.539(3)	C(47)-C(48)	1.385(4)
C(18)-C(19)	1.539(3)	C(48)-C(49)	1.395(4)
C(18)-C(21)	1.535(3)	C(50)-C(51)	1.382(3)
C(18)-C(20)	1.542(3)	C(50)-C(55)	1.398(3)
C(22)-C(23)	1.531(3)	C(51)-C(52)	1.381(3)
C(22)-C(25)	1.526(4)	C(52)-C(53)	1.397(4)
C(22)-C(24)	1.526(3)	C(53)-C(54)	1.369(4)

C(54)-C(55)	1.383(3)	N(1)-Ir(1)-P(1)	94.03(4)
C(56)-C(57)	1.389(3)	O(1)-Ir(1)-P(2)	81.03(4)
C(56)-C(61)	1.388(3)	O(2)-Ir(1)-P(2)	95.07(4)
C(57)-C(58)	1.392(4)	C(73)-Ir(1)-P(2)	68.10(6)
C(58)-C(59)	1.367(4)	N(1)-Ir(1)-P(2)	102.13(4)
C(59)-C(60)	1.381(4)	P(1)-Ir(1)-P(2)	163.84(2)
C(60)-C(61)	1.378(4)	C(50)-P(1)-C(44)	104.99(11)
C(62)-C(67)	1.384(3)	C(50)-P(1)-C(38)	101.32(9)
C(62)-C(63)	1.390(3)	C(44)-P(1)-C(38)	100.02(10)
C(63)-C(64)	1.389(3)	C(50)-P(1)-Ir(1)	114.47(7)
C(64)-C(65)	1.389(3)	C(44)-P(1)-Ir(1)	120.06(6)
C(65)-C(66)	1.376(3)	C(38)-P(1)-Ir(1)	113.48(7)
C(66)-C(67)	1.390(3)	C(68)-P(2)-C(62)	111.29(10)
C(68)-C(69)	1.386(3)	C(68)-P(2)-C(56)	108.28(11)
C(68)-C(73)	1.415(3)	C(62)-P(2)-C(56)	105.07(10)
C(69)-C(70)	1.379(3)	C(68)-P(2)-Ir(1)	84.16(7)
C(70)-C(71)	1.382(3)	C(62)-P(2)-Ir(1)	118.82(7)
C(71)-C(72)	1.392(3)	C(56)-P(2)-Ir(1)	126.24(6)
C(72)-C(73)	1.394(3)	C(1)-O(1)-Ir(1)	121.07(12)
		C(17)-O(2)-Ir(1)	120.12(13)
O(1)-Ir(1)-O(2)	175.07(6)	C(11)-N(1)-C(7)	119.66(19)
O(1)-Ir(1)-C(73)	80.87(7)	C(11)-N(1)-Ir(1)	121.10(15)
O(2)-Ir(1)-C(73)	100.54(7)	C(7)-N(1)-Ir(1)	119.23(15)
O(1)-Ir(1)-N(1)	89.03(6)	O(1)-C(1)-C(6)	123.05(19)
O(2)-Ir(1)-N(1)	88.85(6)	O(1)-C(1)-C(2)	118.83(18)
C(73)-Ir(1)-N(1)	166.84(6)	C(6)-C(1)-C(2)	118.1(2)
O(1)-Ir(1)-P(1)	99.46(4)	C(3)-C(2)-C(1)	118.63(19)
O(2)-Ir(1)-P(1)	85.13(4)	C(3)-C(2)-C(18)	120.9(2)
C(73)-Ir(1)-P(1)	95.93(6)	C(1)-C(2)-C(18)	120.49(19)

C(2)-C(3)-C(4)	123.6(2)	C(17)-C(16)-C(34)	121.0(2)
C(5)-C(4)-C(3)	116.0(2)	O(2)-C(17)-C(12)	123.9(2)
C(5)-C(4)-C(22)	121.62(19)	O(2)-C(17)-C(16)	118.3(2)
C(3)-C(4)-C(22)	122.3(2)	C(12)-C(17)-C(16)	117.7(2)
C(4)-C(5)-C(6)	123.8(2)	C(19)-C(18)-C(21)	109.7(2)
C(5)-C(6)-C(1)	118.4(2)	C(19)-C(18)-C(2)	111.37(17)
C(5)-C(6)-C(7)	117.25(19)	C(21)-C(18)-C(2)	108.53(19)
C(1)-C(6)-C(7)	123.94(19)	C(19)-C(18)-C(20)	107.3(2)
N(1)-C(7)-C(8)	119.7(2)	C(21)-C(18)-C(20)	107.98(19)
N(1)-C(7)-C(6)	122.9(2)	C(2)-C(18)-C(20)	111.84(19)
C(8)-C(7)-C(6)	117.4(2)	C(23)-C(22)-C(4)	108.6(2)
C(7)-C(8)-C(9)	121.9(2)	C(23)-C(22)-C(25)	109.36(19)
C(10)-C(9)-C(8)	116.1(2)	C(4)-C(22)-C(25)	110.0(2)
C(10)-C(9)-C(26)	121.7(2)	C(23)-C(22)-C(24)	108.4(2)
C(8)-C(9)-C(26)	122.1(2)	C(4)-C(22)-C(24)	113.14(18)
C(9)-C(10)-C(11)	122.3(2)	C(25)-C(22)-C(24)	107.3(2)
N(1)-C(11)-C(10)	119.6(2)	C(28)-C(26)-C(27)	108.1(2)
N(1)-C(11)-C(12)	122.5(2)	C(28)-C(26)-C(29)	108.7(2)
C(10)-C(11)-C(12)	117.8(2)	C(27)-C(26)-C(29)	108.9(2)
C(13)-C(12)-C(17)	119.8(2)	C(28)-C(26)-C(9)	113.1(2)
C(13)-C(12)-C(11)	115.5(2)	C(27)-C(26)-C(9)	106.70(19)
C(17)-C(12)-C(11)	124.1(2)	C(29)-C(26)-C(9)	111.24(18)
C(14)-C(13)-C(12)	123.3(2)	C(31A)-C(30)-C(33B)	127.4(7)
C(13)-C(14)-C(15)	115.9(2)	C(31A)-C(30)-C(14)	111.9(5)
C(13)-C(14)-C(30)	122.6(2)	C(33B)-C(30)-C(14)	113.7(4)
C(15)-C(14)-C(30)	121.3(2)	C(31A)-C(30)-C(32A)	115.1(9)
C(16)-C(15)-C(14)	124.3(2)	C(33B)-C(30)-C(32A)	23.1(10)
C(15)-C(16)-C(17)	118.6(2)	C(14)-C(30)-C(32A)	109.2(6)
C(15)-C(16)-C(34)	120.2(2)	C(31A)-C(30)-C(31B)	74.3(7)

C(33B)-C(30)-C(31B)	109.0(6)	C(49)-C(44)-P(1)	121.49(19)
C(14)-C(30)-C(31B)	113.5(3)	C(45)-C(44)-P(1)	120.78(19)
C(32A)-C(30)-C(31B)	128.1(7)	C(44)-C(45)-C(46)	121.4(3)
C(31A)-C(30)-C(33A)	112.0(7)	C(47)-C(46)-C(45)	119.8(3)
C(33B)-C(30)-C(33A)	75.6(6)	C(46)-C(47)-C(48)	120.0(3)
C(14)-C(30)-C(33A)	109.3(3)	C(49)-C(48)-C(47)	119.9(3)
C(32A)-C(30)-C(33A)	98.5(7)	C(48)-C(49)-C(44)	121.1(3)
C(31B)-C(30)-C(33A)	40.1(3)	C(51)-C(50)-C(55)	119.3(2)
C(31A)-C(30)-C(32B)	32.6(9)	C(51)-C(50)-P(1)	123.72(19)
C(33B)-C(30)-C(32B)	106.5(6)	C(55)-C(50)-P(1)	117.01(17)
C(14)-C(30)-C(32B)	108.6(4)	C(52)-C(51)-C(50)	119.8(2)
C(32A)-C(30)-C(32B)	87.5(7)	C(51)-C(52)-C(53)	120.2(3)
C(31B)-C(30)-C(32B)	105.0(5)	C(54)-C(53)-C(52)	120.5(2)
C(33A)-C(30)-C(32B)	137.0(5)	C(53)-C(54)-C(55)	119.2(2)
C(37)-C(34)-C(35)	105.90(19)	C(54)-C(55)-C(50)	121.0(2)
C(37)-C(34)-C(16)	111.94(17)	C(57)-C(56)-C(61)	119.0(3)
C(35)-C(34)-C(16)	112.9(2)	C(57)-C(56)-P(2)	121.0(2)
C(37)-C(34)-C(36)	111.5(2)	C(61)-C(56)-P(2)	119.9(2)
C(35)-C(34)-C(36)	107.24(18)	C(56)-C(57)-C(58)	120.3(3)
C(16)-C(34)-C(36)	107.33(18)	C(59)-C(58)-C(57)	120.2(3)
C(39)-C(38)-C(43)	119.1(2)	C(58)-C(59)-C(60)	119.5(3)
C(39)-C(38)-P(1)	120.33(15)	C(61)-C(60)-C(59)	121.1(3)
C(43)-C(38)-P(1)	120.14(18)	C(60)-C(61)-C(56)	119.9(3)
C(40)-C(39)-C(38)	120.63(19)	C(67)-C(62)-C(63)	119.0(2)
C(39)-C(40)-C(41)	120.3(2)	C(67)-C(62)-P(2)	119.50(15)
C(42)-C(41)-C(40)	119.2(2)	C(63)-C(62)-P(2)	121.46(18)
C(43)-C(42)-C(41)	121.0(2)	C(64)-C(63)-C(62)	120.2(2)
C(42)-C(43)-C(38)	119.8(2)	C(65)-C(64)-C(63)	120.1(2)
C(49)-C(44)-C(45)	117.7(2)	C(64)-C(65)-C(66)	119.9(2)

C(65)-C(66)-C(67)	119.8(2)
C(62)-C(67)-C(66)	120.93(19)
C(69)-C(68)-C(73)	123.4(2)
C(69)-C(68)-P(2)	135.19(17)
C(73)-C(68)-P(2)	101.27(15)
C(70)-C(69)-C(68)	118.0(2)
C(69)-C(70)-C(71)	120.5(2)
C(72)-C(71)-C(70)	121.0(2)
C(71)-C(72)-C(73)	120.6(2)
C(72)-C(73)-C(68)	116.38(19)
C(72)-C(73)-Ir(1)	136.70(16)
C(68)-C(73)-Ir(1)	105.26(15)

Table S65. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **18**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	124(1)	150(1)	94(1)	5(1)	46(1)	14(1)
P(1)	170(3)	158(3)	108(2)	-2(2)	43(2)	10(2)
P(2)	158(3)	175(3)	109(2)	-3(2)	57(2)	15(2)
O(1)	178(9)	169(8)	129(6)	35(6)	75(6)	32(7)
O(2)	158(9)	142(8)	125(6)	14(6)	41(6)	6(7)
N(1)	150(10)	161(9)	86(7)	-16(7)	50(7)	-1(9)
C(1)	135(12)	176(12)	113(9)	-7(8)	32(9)	-3(9)
C(2)	144(13)	187(12)	153(9)	17(9)	50(9)	5(9)
C(3)	177(13)	185(12)	178(10)	27(9)	42(9)	10(10)
C(4)	193(14)	201(13)	165(10)	8(9)	61(9)	40(10)
C(5)	197(13)	206(13)	164(9)	9(9)	100(9)	44(10)
C(6)	163(13)	169(12)	119(9)	12(8)	53(9)	11(9)
C(7)	171(13)	167(12)	91(8)	-7(8)	58(9)	8(9)
C(8)	170(13)	206(13)	157(9)	19(9)	75(9)	66(10)
C(9)	155(12)	227(12)	130(8)	-12(10)	65(8)	11(11)
C(10)	176(13)	185(12)	134(9)	11(8)	67(9)	-15(10)
C(11)	144(12)	182(12)	72(8)	-15(8)	28(8)	-9(9)
C(12)	160(13)	174(11)	91(8)	-2(8)	54(9)	15(9)
C(13)	167(13)	200(12)	116(9)	-6(8)	34(9)	-6(10)
C(14)	219(14)	201(13)	128(9)	-5(9)	32(9)	-11(10)
C(15)	247(14)	155(12)	156(9)	8(9)	65(10)	12(10)
C(16)	182(13)	176(12)	125(9)	-2(8)	67(9)	20(10)
C(17)	182(13)	147(11)	93(8)	-16(8)	71(9)	-1(9)
C(18)	229(14)	210(13)	227(11)	71(9)	121(10)	51(10)

C(19)	241(16)	418(18)	394(14)	102(13)	194(13)	24(13)
C(20)	470(20)	292(16)	447(15)	148(13)	344(15)	89(14)
C(21)	429(18)	367(16)	202(11)	7(11)	193(12)	-1(14)
C(22)	307(16)	195(13)	240(11)	9(9)	143(11)	59(11)
C(23)	402(18)	314(16)	394(14)	-159(13)	162(13)	5(14)
C(24)	800(30)	244(16)	468(16)	87(13)	409(18)	209(16)
C(25)	323(18)	280(16)	447(15)	-62(12)	163(14)	91(13)
C(26)	181(13)	293(13)	206(10)	39(11)	108(9)	38(12)
C(27)	283(18)	870(30)	302(13)	-148(15)	178(13)	31(17)
C(28)	311(19)	356(18)	760(20)	70(16)	363(17)	21(14)
C(29)	205(16)	530(20)	398(14)	168(14)	151(13)	92(14)
C(30)	266(16)	192(13)	248(11)	15(10)	15(11)	-46(11)
C(31A)	1640(190)	590(90)	590(80)	-390(70)	790(110)	-840(100)
C(32A)	410(60)	60(40)	1930(170)	-190(70)	110(90)	-80(40)
C(33A)	210(50)	390(50)	480(50)	-20(40)	40(30)	-120(40)
C(31B)	280(40)	400(40)	1110(80)	310(40)	-70(40)	-120(30)
C(32B)	680(60)	550(60)	280(30)	60(30)	140(30)	-350(40)
C(33B)	1830(160)	810(90)	1430(100)	-910(80)	1480(120)	-990(90)
C(34)	175(14)	198(13)	205(10)	32(9)	63(10)	24(10)
C(35)	229(15)	230(14)	381(13)	82(11)	44(12)	56(11)
C(36)	198(14)	287(14)	149(9)	50(9)	13(9)	-19(10)
C(37)	210(15)	261(14)	297(12)	6(11)	113(11)	49(11)
C(38)	146(12)	173(12)	131(9)	16(8)	17(9)	-16(9)
C(39)	190(14)	205(13)	148(9)	14(9)	42(9)	-4(10)
C(40)	166(14)	223(13)	242(11)	25(10)	60(10)	13(10)
C(41)	191(14)	294(14)	179(10)	58(10)	0(10)	-24(11)
C(42)	254(15)	343(16)	135(9)	7(10)	20(9)	-27(12)
C(43)	221(14)	270(14)	140(9)	-6(9)	55(10)	2(11)
C(44)	217(14)	195(12)	147(9)	-17(9)	61(9)	-26(10)

C(45)	276(16)	241(14)	195(11)	-13(10)	48(10)	-35(11)
C(46)	430(20)	236(15)	290(13)	54(11)	38(13)	-43(13)
C(47)	460(20)	254(16)	490(16)	56(13)	95(15)	-160(14)
C(48)	298(18)	347(18)	484(16)	51(14)	-4(14)	-133(14)
C(49)	279(16)	239(14)	315(12)	31(11)	65(11)	-26(12)
C(50)	186(13)	229(13)	85(8)	5(8)	38(9)	56(10)
C(51)	457(19)	233(14)	278(12)	11(11)	228(13)	49(13)
C(52)	670(20)	279(16)	461(15)	21(13)	393(17)	172(16)
C(53)	408(19)	510(20)	280(13)	68(13)	241(13)	178(15)
C(54)	259(15)	361(16)	169(10)	22(10)	103(10)	38(12)
C(55)	209(14)	258(13)	114(9)	-6(9)	52(9)	47(10)
C(56)	317(14)	204(12)	118(8)	-4(10)	98(9)	25(12)
C(57)	378(19)	283(16)	368(14)	-31(12)	117(13)	80(13)
C(58)	660(30)	295(18)	480(17)	-16(14)	134(17)	228(17)
C(59)	1000(30)	183(16)	313(14)	-3(12)	215(18)	56(18)
C(60)	820(30)	277(17)	327(14)	-121(12)	331(17)	-216(17)
C(61)	451(19)	283(15)	248(12)	-102(11)	209(13)	-102(13)
C(62)	180(13)	178(12)	119(9)	-5(8)	48(9)	-6(10)
C(63)	226(15)	310(14)	153(10)	-26(10)	78(10)	8(11)
C(64)	323(16)	302(15)	130(9)	-6(10)	64(10)	8(12)
C(65)	273(15)	218(13)	163(9)	12(10)	-1(9)	15(12)
C(66)	180(13)	265(13)	220(10)	7(11)	45(9)	19(11)
C(67)	217(14)	226(13)	176(10)	5(9)	87(10)	0(10)
C(68)	127(12)	215(12)	150(9)	38(9)	55(9)	37(9)
C(69)	168(14)	346(15)	144(9)	27(9)	70(9)	50(11)
C(70)	163(14)	475(18)	188(10)	83(10)	106(10)	36(12)
C(71)	136(13)	331(15)	246(11)	73(10)	68(10)	7(11)
C(72)	158(13)	235(13)	173(10)	23(9)	41(9)	20(10)
C(73)	155(12)	154(11)	155(9)	39(9)	59(8)	46(10)

[(ONO^{tBu})Ir(PPh$_3$)CH$_2$CN]$_2$, 19

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The solvent occupied area of the crystal comprises 25.3% (1518.8Å3) of the total unit cell volume. We were unable to obtain a satisfactory model for this region. Therefore the observed intensities were adjusted to remove contribution to the electron density map using the program SQUEEZE[iii]. A total of 278 electrons were accounted for which in close agreement with the 291 electrons expected for two molecules of di-n-butyl ether per asymmetric unit.

The Li atoms were fixed at the positions derived from the electron density map and the isotropic displacement parameters were manually adjusted to flatten the electron density difference map and were also fixed during refinement. As a side effect of the solvent flattening routine it is not possible to fully define the overall charge balance as any counterion to Li would be removed from the model.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S66. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **19**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ir(1)	9414(1)	6430(1)	7990(1)	17(1)	1
Ir(2)	7883(1)	8586(1)	7127(1)	19(1)	1
P(1)	10305(1)	5616(1)	7812(1)	19(1)	1
P(2)	7039(1)	9414(1)	7366(1)	23(1)	1
O(1)	10154(1)	6922(1)	8816(1)	21(1)	1
O(2)	8598(1)	6042(1)	7216(1)	19(1)	1

O(3)	8752(1)	9541(1)	6918(1)	22(1)	1
O(4)	7099(1)	7580(1)	7292(1)	22(1)	1
N(1)	8670(1)	5659(1)	8487(1)	17(1)	1
N(2)	7431(1)	8366(1)	6189(1)	22(1)	1
N(3)	8702(1)	7276(1)	8180(1)	18(1)	1
N(4)	8800(1)	7916(1)	6991(1)	18(1)	1
C(1)	9722(2)	7159(1)	9255(1)	21(1)	1
C(2)	10003(2)	7914(1)	9603(1)	24(1)	1
C(3)	9483(2)	8170(1)	9998(1)	28(1)	1
C(4)	8697(2)	7742(1)	10086(1)	26(1)	1
C(5)	8469(2)	6991(1)	9778(1)	24(1)	1
C(6)	8969(2)	6689(1)	9382(1)	20(1)	1
C(7)	8622(2)	5872(1)	9095(1)	18(1)	1
C(8)	8209(2)	5336(1)	9459(1)	22(1)	1
C(9)	7752(2)	4607(1)	9202(1)	23(1)	1
C(10)	7741(2)	4438(1)	8568(1)	22(1)	1
C(11)	8219(2)	4954(1)	8213(1)	18(1)	1
C(12)	8167(2)	4732(1)	7539(1)	18(1)	1
C(13)	7926(2)	3923(1)	7331(1)	21(1)	1
C(14)	7693(2)	3642(1)	6719(1)	23(1)	1
C(15)	7673(2)	4219(1)	6287(1)	24(1)	1
C(16)	7940(2)	5020(1)	6448(1)	20(1)	1
C(17)	8254(2)	5290(1)	7081(1)	18(1)	1
C(18)	10840(2)	8447(1)	9520(1)	29(1)	1
C(19)	10799(2)	8703(1)	8854(1)	35(1)	1
C(20)	11553(2)	8004(1)	9646(1)	33(1)	1
C(21)	11051(2)	9206(1)	9966(1)	39(1)	1
C(22)	8108(2)	8082(1)	10469(1)	35(1)	1
C(23)	7636(3)	8564(3)	10026(2)	59(2)	0.740(5)

C(24)	8583(3)	8661(3)	11001(2)	59(2)	0.740(5)
C(25)	7499(5)	7450(3)	10706(3)	101(3)	0.740(5)
C(23B)	7280(12)	7615(10)	10413(8)	59(5)	0.260(5)
C(24B)	8388(8)	7970(7)	11217(5)	47(4)	0.260(5)
C(25B)	8100(10)	8911(8)	10466(7)	63(4)	0.260(5)
C(26)	7277(2)	4051(1)	9617(1)	32(1)	1
C(27)	6625(2)	4439(2)	9884(2)	51(1)	1
C(28)	7909(2)	3921(2)	10165(1)	54(1)	1
C(29)	6896(3)	3248(2)	9279(2)	75(1)	1
C(30)	7446(2)	2751(1)	6524(1)	30(1)	1
C(31)	6659(2)	2403(2)	6807(1)	37(1)	1
C(32)	8167(2)	2351(1)	6751(1)	38(1)	1
C(33)	7265(2)	2573(2)	5815(1)	49(1)	1
C(34)	7927(2)	5615(1)	5946(1)	25(1)	1
C(35)	8816(2)	6045(2)	5875(1)	30(1)	1
C(36)	7543(2)	5202(2)	5310(1)	34(1)	1
C(37)	7406(2)	6224(1)	6121(1)	28(1)	1
C(38)	10334(2)	5254(1)	7005(1)	24(1)	1
C(39)	10928(2)	5665(2)	6668(1)	31(1)	1
C(40)	10960(2)	5413(2)	6056(1)	44(1)	1
C(41)	10425(2)	4733(2)	5772(1)	44(1)	1
C(42)	9831(2)	4335(2)	6097(1)	34(1)	1
C(43)	9778(2)	4593(1)	6704(1)	27(1)	1
C(44)	11416(2)	6042(1)	8055(1)	22(1)	1
C(45)	11711(2)	6842(1)	8230(1)	25(1)	1
C(46)	12556(2)	7135(2)	8400(1)	30(1)	1
C(47)	13113(2)	6637(2)	8406(1)	31(1)	1
C(48)	12831(2)	5839(2)	8234(1)	32(1)	1
C(49)	11991(2)	5540(2)	8060(1)	30(1)	1

C(50)	10190(2)	4745(1)	8261(1)	20(1)	1
C(51)	10149(2)	4892(1)	8892(1)	21(1)	1
C(52)	10088(2)	4277(1)	9277(1)	24(1)	1
C(53)	10080(2)	3517(1)	9034(1)	30(1)	1
C(54)	10136(2)	3370(1)	8412(1)	32(1)	1
C(55)	10191(2)	3977(1)	8023(1)	25(1)	1
C(56)	8517(2)	7873(1)	8185(1)	19(1)	1
C(57)	8311(2)	8640(1)	8099(1)	22(1)	1
C(58)	9207(2)	9387(1)	6467(1)	22(1)	1
C(59)	10069(2)	9749(1)	6516(1)	24(1)	1
C(60)	10543(2)	9500(1)	6081(1)	28(1)	1
C(61)	10226(2)	8918(1)	5587(1)	26(1)	1
C(62)	9373(2)	8640(1)	5517(1)	26(1)	1
C(63)	8858(2)	8877(1)	5930(1)	22(1)	1
C(64)	7955(2)	8586(1)	5756(1)	23(1)	1
C(65)	7637(2)	8532(1)	5136(1)	28(1)	1
C(66)	6821(2)	8197(2)	4929(1)	32(1)	1
C(67)	6335(2)	7901(2)	5371(1)	31(1)	1
C(68)	6631(2)	8004(1)	6003(1)	24(1)	1
C(69)	6059(2)	7683(1)	6444(1)	26(1)	1
C(70)	5200(2)	7571(2)	6252(1)	34(1)	1
C(71)	4600(2)	7142(2)	6548(1)	40(1)	1
C(72)	4890(2)	6762(2)	7061(1)	35(1)	1
C(73)	5716(2)	6870(1)	7297(1)	27(1)	1
C(74)	6325(2)	7395(1)	7019(1)	24(1)	1
C(75)	10469(2)	10367(2)	7054(1)	30(1)	1
C(76)	10460(2)	9962(2)	7669(1)	36(1)	1
C(77)	11383(2)	10733(2)	7001(1)	49(1)	1
C(78)	9996(2)	11055(1)	7071(1)	36(1)	1

C(79)	10791(2)	8627(2)	5158(1)	33(1)	1
C(80)	11508(3)	8365(3)	5517(2)	95(2)	1
C(81)	11109(2)	9276(2)	4749(2)	58(1)	1
C(82)	10315(3)	7917(2)	4683(2)	67(1)	1
C(83)	6485(2)	8153(2)	4237(1)	53(1)	1
C(84)	6934(3)	7652(3)	3868(2)	99(2)	1
C(85)	6745(3)	9023(2)	4012(2)	76(1)	1
C(86)	5575(2)	7959(3)	4122(2)	93(2)	1
C(87)	3670(2)	7056(3)	6330(2)	66(1)	1
C(88)	3479(4)	7106(4)	5681(3)	55(2)	0.557(5)
C(89)	3241(5)	7428(5)	6764(4)	83(2)	0.557(5)
C(90)	3237(5)	6056(4)	6377(4)	89(3)	0.557(5)
C(88B)	3428(6)	6543(6)	5728(4)	75(3)	0.443(5)
C(89B)	3130(5)	6872(5)	6763(3)	48(2)	0.443(5)
C(90B)	3550(6)	7900(5)	6026(4)	81(3)	0.443(5)
C(91)	5996(2)	6447(2)	7869(1)	32(1)	1
C(92)	5256(2)	5862(2)	8068(1)	44(1)	1
C(93)	6359(2)	7042(2)	8429(1)	36(1)	1
C(94)	6644(2)	5965(2)	7701(1)	35(1)	1
C(95)	6272(2)	9099(2)	7899(1)	29(1)	1
C(96)	6490(2)	9322(2)	8538(1)	38(1)	1
C(97)	5928(2)	9097(2)	8957(2)	51(1)	1
C(98)	5140(2)	8658(2)	8746(2)	57(1)	1
C(99)	4921(2)	8431(2)	8127(2)	48(1)	1
C(100)	5487(2)	8639(2)	7704(1)	36(1)	1
C(101)	7557(2)	10378(1)	7772(1)	25(1)	1
C(102)	8396(2)	10571(1)	7992(1)	27(1)	1
C(103)	8735(2)	11292(1)	8335(1)	30(1)	1
C(104)	8234(2)	11820(2)	8466(1)	37(1)	1

C(105)	7391(2)	11630(2)	8248(1)	38(1)	1
C(106)	7054(2)	10921(2)	7904(1)	34(1)	1
C(107)	6487(2)	9755(1)	6690(1)	24(1)	1
C(108)	6987(2)	10010(1)	6236(1)	26(1)	1
C(109)	6637(2)	10296(1)	5700(1)	31(1)	1
C(110)	5808(2)	10334(2)	5633(1)	36(1)	1
C(111)	5321(2)	10095(2)	6087(1)	43(1)	1
C(112)	5662(2)	9808(2)	6619(1)	32(1)	1
C(113)	9346(2)	7623(1)	7123(1)	20(1)	1
C(114)	10000(2)	7233(1)	7380(1)	22(1)	1
Li(1)	10967	4295	8861	100	1
Li(2)	6387	10760	6278	100	1

Table S67. Selected bond lengths [Å] and angles [°] for **19**.

Ir(1)-O(2)	2.0228(15)	O(2)-Ir(1)-N(1)	89.49(7)
Ir(1)-N(1)	2.0719(18)	O(2)-Ir(1)-O(1)	172.83(6)
Ir(1)-O(1)	2.0867(15)	N(1)-Ir(1)-O(1)	89.51(7)
Ir(1)-N(3)	2.089(2)	O(2)-Ir(1)-N(3)	87.82(7)
Ir(1)-C(114)	2.152(2)	N(1)-Ir(1)-N(3)	88.73(7)
Ir(1)-P(1)	2.2644(7)	O(1)-Ir(1)-N(3)	85.06(7)
Ir(2)-O(4)	2.0335(15)	O(2)-Ir(1)-C(114)	82.38(8)
Ir(2)-N(2)	2.0780(19)	N(1)-Ir(1)-C(114)	170.69(8)
Ir(2)-O(3)	2.0750(15)	O(1)-Ir(1)-C(114)	97.99(8)
Ir(2)-N(4)	2.105(2)	N(3)-Ir(1)-C(114)	86.45(8)
Ir(2)-C(57)	2.147(2)	O(2)-Ir(1)-P(1)	96.58(5)
Ir(2)-P(2)	2.2525(7)	N(1)-Ir(1)-P(1)	95.47(5)
		O(1)-Ir(1)-P(1)	90.58(5)
		N(3)-Ir(1)-P(1)	173.92(6)
		C(114)-Ir(1)-P(1)	89.98(7)
		O(4)-Ir(2)-N(2)	89.33(7)
		O(4)-Ir(2)-O(3)	174.40(7)
		N(2)-Ir(2)-O(3)	88.96(7)
		O(4)-Ir(2)-N(4)	89.08(7)
		N(2)-Ir(2)-N(4)	89.96(7)
		O(3)-Ir(2)-N(4)	85.59(7)
		O(4)-Ir(2)-C(57)	83.83(7)
		N(2)-Ir(2)-C(57)	172.15(7)
		O(3)-Ir(2)-C(57)	97.48(8)
		N(4)-Ir(2)-C(57)	86.09(8)
		O(4)-Ir(2)-P(2)	95.85(5)
		N(2)-Ir(2)-P(2)	96.37(6)

O(3)-Ir(2)-P(2)	89.64(5)	C(57)-Ir(2)-P(2)	88.18(7)
N(4)-Ir(2)-P(2)	172.00(6)		

Table S68. Bond lengths [Å] and angles [°] for **19**.

Ir(1)-O(2)	2.0228(15)	N(1)-C(7)	1.362(3)
Ir(1)-N(1)	2.0719(18)	N(2)-C(68)	1.348(3)
Ir(1)-O(1)	2.0867(15)	N(2)-C(64)	1.368(3)
Ir(1)-N(3)	2.089(2)	N(3)-C(56)	1.131(3)
Ir(1)-C(114)	2.152(2)	N(4)-C(113)	1.135(3)
Ir(1)-P(1)	2.2644(7)	C(1)-C(6)	1.409(3)
Ir(2)-O(4)	2.0335(15)	C(1)-C(2)	1.430(3)
Ir(2)-N(2)	2.0780(19)	C(2)-C(3)	1.385(4)
Ir(2)-O(3)	2.0750(15)	C(2)-C(18)	1.537(4)
Ir(2)-N(4)	2.105(2)	C(3)-C(4)	1.399(4)
Ir(2)-C(57)	2.147(2)	C(4)-C(5)	1.383(3)
Ir(2)-P(2)	2.2525(7)	C(4)-C(22)	1.517(4)
P(1)-C(38)	1.831(3)	C(5)-C(6)	1.396(3)
P(1)-C(44)	1.837(3)	C(6)-C(7)	1.483(3)
P(1)-C(50)	1.840(2)	C(7)-C(8)	1.386(3)
P(2)-C(101)	1.834(3)	C(8)-C(9)	1.382(3)
P(2)-C(107)	1.836(2)	C(9)-C(10)	1.389(3)
P(2)-C(95)	1.838(3)	C(9)-C(26)	1.525(3)
O(1)-C(1)	1.337(3)	C(10)-C(11)	1.402(3)
O(2)-C(17)	1.313(3)	C(11)-C(12)	1.480(3)
O(3)-C(58)	1.339(3)	C(12)-C(13)	1.405(3)
O(4)-C(74)	1.315(3)	C(12)-C(17)	1.433(3)
N(1)-C(11)	1.358(3)	C(13)-C(14)	1.372(3)

C(14)-C(15)	1.418(3)	C(44)-C(45)	1.386(3)
C(14)-C(30)	1.533(3)	C(44)-C(49)	1.403(3)
C(15)-C(16)	1.378(3)	C(45)-C(46)	1.385(3)
C(16)-C(17)	1.429(3)	C(46)-C(47)	1.373(4)
C(16)-C(34)	1.553(3)	C(47)-C(48)	1.378(4)
C(18)-C(21)	1.535(4)	C(48)-C(49)	1.380(4)
C(18)-C(19)	1.543(3)	C(50)-C(51)	1.390(3)
C(18)-C(20)	1.533(4)	C(50)-C(55)	1.392(3)
C(22)-C(25B)	1.435(13)	C(51)-C(52)	1.394(3)
C(22)-C(25)	1.494(6)	C(52)-C(53)	1.380(3)
C(22)-C(24)	1.515(5)	C(53)-C(54)	1.375(4)
C(22)-C(23)	1.557(5)	C(54)-C(55)	1.389(3)
C(22)-C(23B)	1.431(19)	C(56)-C(57)	1.450(3)
C(22)-C(24B)	1.679(11)	C(58)-C(63)	1.409(3)
C(26)-C(27)	1.517(4)	C(58)-C(59)	1.425(3)
C(26)-C(29)	1.510(4)	C(59)-C(60)	1.386(4)
C(26)-C(28)	1.555(4)	C(59)-C(75)	1.527(4)
C(30)-C(32)	1.540(4)	C(60)-C(61)	1.401(4)
C(30)-C(33)	1.535(3)	C(61)-C(62)	1.382(4)
C(30)-C(31)	1.529(4)	C(61)-C(79)	1.513(4)
C(34)-C(36)	1.525(3)	C(62)-C(63)	1.393(4)
C(34)-C(37)	1.534(4)	C(63)-C(64)	1.471(3)
C(34)-C(35)	1.536(4)	C(64)-C(65)	1.384(3)
C(38)-C(43)	1.391(3)	C(65)-C(66)	1.369(4)
C(38)-C(39)	1.399(3)	C(66)-C(67)	1.379(4)
C(39)-C(40)	1.382(4)	C(66)-C(83)	1.537(4)
C(40)-C(41)	1.385(4)	C(67)-C(68)	1.396(3)
C(41)-C(42)	1.374(4)	C(68)-C(69)	1.477(4)
C(42)-C(43)	1.380(4)	C(69)-C(70)	1.403(4)

C(69)-C(74)	1.433(3)	C(98)-C(99)	1.366(5)
C(70)-C(71)	1.362(4)	C(99)-C(100)	1.394(4)
C(71)-C(72)	1.419(3)	C(101)-C(102)	1.380(4)
C(71)-C(87)	1.529(4)	C(101)-C(106)	1.402(4)
C(72)-C(73)	1.372(4)	C(102)-C(103)	1.391(3)
C(73)-C(74)	1.431(3)	C(103)-C(104)	1.378(4)
C(73)-C(91)	1.558(3)	C(104)-C(105)	1.383(4)
C(75)-C(77)	1.534(4)	C(105)-C(106)	1.375(4)
C(75)-C(78)	1.542(4)	C(107)-C(112)	1.371(4)
C(75)-C(76)	1.554(3)	C(107)-C(108)	1.395(4)
C(79)-C(80)	1.505(4)	C(108)-C(109)	1.406(3)
C(79)-C(81)	1.527(3)	C(109)-C(110)	1.372(4)
C(79)-C(82)	1.571(4)	C(110)-C(111)	1.375(4)
C(83)-C(86)	1.460(5)	C(111)-C(112)	1.396(3)
C(83)-C(84)	1.490(5)	C(113)-C(114)	1.458(3)
C(83)-C(85)	1.606(5)		
C(87)-C(89B)	1.373(8)	O(2)-Ir(1)-N(1)	89.49(7)
C(87)-C(88)	1.426(6)	O(2)-Ir(1)-O(1)	172.83(6)
C(87)-C(89)	1.428(8)	N(1)-Ir(1)-O(1)	89.51(7)
C(87)-C(88B)	1.501(10)	O(2)-Ir(1)-N(3)	87.82(7)
C(87)-C(90)	1.752(8)	N(1)-Ir(1)-N(3)	88.73(7)
C(87)-C(90B)	1.680(8)	O(1)-Ir(1)-N(3)	85.06(7)
C(91)-C(94)	1.533(4)	O(2)-Ir(1)-C(114)	82.38(8)
C(91)-C(93)	1.528(4)	N(1)-Ir(1)-C(114)	170.69(8)
C(91)-C(92)	1.545(4)	O(1)-Ir(1)-C(114)	97.99(8)
C(95)-C(100)	1.384(4)	N(3)-Ir(1)-C(114)	86.45(8)
C(95)-C(96)	1.403(4)	O(2)-Ir(1)-P(1)	96.58(5)
C(96)-C(97)	1.390(4)	N(1)-Ir(1)-P(1)	95.47(5)
C(97)-C(98)	1.382(5)	O(1)-Ir(1)-P(1)	90.58(5)

N(3)-Ir(1)-P(1)	173.92(6)	C(1)-O(1)-Ir(1)	113.77(14)
C(114)-Ir(1)-P(1)	89.98(7)	C(17)-O(2)-Ir(1)	121.94(12)
O(4)-Ir(2)-N(2)	89.33(7)	C(58)-O(3)-Ir(2)	115.58(13)
O(4)-Ir(2)-O(3)	174.40(7)	C(74)-O(4)-Ir(2)	120.99(12)
N(2)-Ir(2)-O(3)	88.96(7)	C(11)-N(1)-C(7)	119.71(19)
O(4)-Ir(2)-N(4)	89.08(7)	C(11)-N(1)-Ir(1)	120.98(15)
N(2)-Ir(2)-N(4)	89.96(7)	C(7)-N(1)-Ir(1)	119.29(14)
O(3)-Ir(2)-N(4)	85.59(7)	C(68)-N(2)-C(64)	119.8(2)
O(4)-Ir(2)-C(57)	83.83(7)	C(68)-N(2)-Ir(2)	120.79(17)
N(2)-Ir(2)-C(57)	172.15(7)	C(64)-N(2)-Ir(2)	119.41(17)
O(3)-Ir(2)-C(57)	97.48(8)	C(56)-N(3)-Ir(1)	157.07(19)
N(4)-Ir(2)-C(57)	86.09(8)	C(113)-N(4)-Ir(2)	157.16(19)
O(4)-Ir(2)-P(2)	95.85(5)	O(1)-C(1)-C(6)	121.8(2)
N(2)-Ir(2)-P(2)	96.37(6)	O(1)-C(1)-C(2)	120.8(2)
O(3)-Ir(2)-P(2)	89.64(5)	C(6)-C(1)-C(2)	117.4(2)
N(4)-Ir(2)-P(2)	172.00(6)	C(3)-C(2)-C(1)	118.3(2)
C(57)-Ir(2)-P(2)	88.18(7)	C(3)-C(2)-C(18)	120.6(2)
C(38)-P(1)-C(44)	100.86(12)	C(1)-C(2)-C(18)	121.1(3)
C(38)-P(1)-C(50)	106.72(11)	C(2)-C(3)-C(4)	124.8(2)
C(44)-P(1)-C(50)	99.39(10)	C(5)-C(4)-C(3)	115.5(3)
C(38)-P(1)-Ir(1)	117.45(8)	C(5)-C(4)-C(22)	121.4(3)
C(44)-P(1)-Ir(1)	115.56(8)	C(3)-C(4)-C(22)	123.0(2)
C(50)-P(1)-Ir(1)	114.55(9)	C(4)-C(5)-C(6)	122.6(2)
C(101)-P(2)-C(107)	99.28(10)	C(5)-C(6)-C(1)	120.9(2)
C(101)-P(2)-C(95)	99.32(13)	C(5)-C(6)-C(7)	114.8(2)
C(107)-P(2)-C(95)	107.59(12)	C(1)-C(6)-C(7)	124.2(2)
C(101)-P(2)-Ir(2)	116.02(9)	N(1)-C(7)-C(8)	120.6(2)
C(107)-P(2)-Ir(2)	114.36(9)	N(1)-C(7)-C(6)	121.73(19)
C(95)-P(2)-Ir(2)	117.79(8)	C(8)-C(7)-C(6)	117.6(2)

C(9)-C(8)-C(7)	121.2(2)	C(25B)-C(22)-C(24)	60.0(6)
C(8)-C(9)-C(10)	116.6(2)	C(25)-C(22)-C(24)	110.3(4)
C(8)-C(9)-C(26)	119.3(2)	C(25B)-C(22)-C(4)	118.5(6)
C(10)-C(9)-C(26)	124.0(2)	C(25)-C(22)-C(4)	112.1(3)
C(9)-C(10)-C(11)	121.7(2)	C(24)-C(22)-C(4)	111.5(3)
N(1)-C(11)-C(10)	119.5(2)	C(25B)-C(22)-C(23)	47.1(6)
N(1)-C(11)-C(12)	122.16(19)	C(25)-C(22)-C(23)	109.9(5)
C(10)-C(11)-C(12)	118.2(2)	C(24)-C(22)-C(23)	106.9(3)
C(13)-C(12)-C(17)	117.9(2)	C(4)-C(22)-C(23)	105.9(3)
C(13)-C(12)-C(11)	117.62(18)	C(25B)-C(22)-C(23B)	111.4(10)
C(17)-C(12)-C(11)	124.13(19)	C(25)-C(22)-C(23B)	31.5(6)
C(14)-C(13)-C(12)	123.83(19)	C(24)-C(22)-C(23B)	129.2(8)
C(13)-C(14)-C(15)	116.4(2)	C(4)-C(22)-C(23B)	114.7(8)
C(13)-C(14)-C(30)	121.08(19)	C(23)-C(22)-C(23B)	79.6(6)
C(15)-C(14)-C(30)	122.5(2)	C(25B)-C(22)-C(24B)	103.9(8)
C(16)-C(15)-C(14)	123.3(2)	C(25)-C(22)-C(24B)	68.2(5)
C(15)-C(16)-C(17)	118.78(19)	C(24)-C(22)-C(24B)	48.0(4)
C(15)-C(16)-C(34)	120.4(2)	C(4)-C(22)-C(24B)	107.8(5)
C(17)-C(16)-C(34)	120.81(19)	C(23)-C(22)-C(24B)	143.9(5)
O(2)-C(17)-C(16)	118.27(18)	C(23B)-C(22)-C(24B)	97.5(8)
O(2)-C(17)-C(12)	123.0(2)	C(27)-C(26)-C(29)	111.7(3)
C(16)-C(17)-C(12)	118.7(2)	C(27)-C(26)-C(9)	109.5(2)
C(2)-C(18)-C(21)	112.9(2)	C(29)-C(26)-C(9)	112.2(2)
C(2)-C(18)-C(19)	109.3(2)	C(27)-C(26)-C(28)	108.0(2)
C(21)-C(18)-C(19)	107.19(19)	C(29)-C(26)-C(28)	107.3(2)
C(2)-C(18)-C(20)	110.17(18)	C(9)-C(26)-C(28)	107.9(2)
C(21)-C(18)-C(20)	106.9(2)	C(32)-C(30)-C(14)	109.3(2)
C(19)-C(18)-C(20)	110.3(2)	C(32)-C(30)-C(33)	107.8(2)
C(25B)-C(22)-C(25)	128.3(7)	C(14)-C(30)-C(33)	112.04(19)

C(32)-C(30)-C(31)	110.1(2)	C(53)-C(52)-C(51)	119.9(2)
C(14)-C(30)-C(31)	109.2(2)	C(54)-C(53)-C(52)	119.8(2)
C(33)-C(30)-C(31)	108.3(2)	C(53)-C(54)-C(55)	120.8(2)
C(36)-C(34)-C(37)	107.7(2)	C(50)-C(55)-C(54)	120.0(2)
C(36)-C(34)-C(35)	106.8(2)	N(3)-C(56)-C(57)	171.6(2)
C(37)-C(34)-C(35)	109.6(2)	C(56)-C(57)-Ir(2)	104.57(16)
C(36)-C(34)-C(16)	111.89(19)	O(3)-C(58)-C(63)	122.0(2)
C(37)-C(34)-C(16)	109.9(2)	O(3)-C(58)-C(59)	120.2(2)
C(35)-C(34)-C(16)	110.84(19)	C(63)-C(58)-C(59)	117.8(2)
C(43)-C(38)-C(39)	117.9(2)	C(60)-C(59)-C(58)	118.4(2)
C(43)-C(38)-P(1)	123.0(2)	C(60)-C(59)-C(75)	120.9(2)
C(39)-C(38)-P(1)	119.1(2)	C(58)-C(59)-C(75)	120.6(2)
C(40)-C(39)-C(38)	120.6(3)	C(59)-C(60)-C(61)	124.2(3)
C(41)-C(40)-C(39)	120.7(3)	C(62)-C(61)-C(60)	115.6(3)
C(42)-C(41)-C(40)	119.0(3)	C(62)-C(61)-C(79)	122.9(3)
C(41)-C(42)-C(43)	120.8(3)	C(60)-C(61)-C(79)	121.5(3)
C(42)-C(43)-C(38)	121.0(3)	C(61)-C(62)-C(63)	122.9(3)
C(45)-C(44)-C(49)	118.4(2)	C(62)-C(63)-C(58)	120.1(2)
C(45)-C(44)-P(1)	122.67(19)	C(62)-C(63)-C(64)	115.9(2)
C(49)-C(44)-P(1)	118.88(18)	C(58)-C(63)-C(64)	123.9(2)
C(44)-C(45)-C(46)	120.4(2)	N(2)-C(64)-C(65)	119.7(2)
C(47)-C(46)-C(45)	120.6(2)	N(2)-C(64)-C(63)	121.8(2)
C(46)-C(47)-C(48)	119.9(2)	C(65)-C(64)-C(63)	118.5(2)
C(49)-C(48)-C(47)	120.2(3)	C(66)-C(65)-C(64)	122.0(3)
C(48)-C(49)-C(44)	120.5(2)	C(65)-C(66)-C(67)	116.3(2)
C(51)-C(50)-C(55)	118.92(19)	C(65)-C(66)-C(83)	120.7(3)
C(51)-C(50)-P(1)	115.96(17)	C(67)-C(66)-C(83)	123.0(3)
C(55)-C(50)-P(1)	125.01(19)	C(66)-C(67)-C(68)	122.1(3)
C(50)-C(51)-C(52)	120.6(2)	N(2)-C(68)-C(67)	119.4(2)

N(2)-C(68)-C(69)	122.3(2)	C(86)-C(83)-C(66)	113.0(3)
C(67)-C(68)-C(69)	118.3(2)	C(84)-C(83)-C(66)	109.5(3)
C(70)-C(69)-C(74)	118.2(2)	C(86)-C(83)-C(85)	105.0(3)
C(70)-C(69)-C(68)	117.3(2)	C(84)-C(83)-C(85)	104.7(3)
C(74)-C(69)-C(68)	124.0(2)	C(66)-C(83)-C(85)	107.6(3)
C(71)-C(70)-C(69)	124.1(2)	C(89B)-C(87)-C(88)	128.6(5)
C(70)-C(71)-C(72)	116.1(3)	C(89B)-C(87)-C(89)	39.2(4)
C(70)-C(71)-C(87)	122.1(2)	C(88)-C(87)-C(89)	120.2(5)
C(72)-C(71)-C(87)	121.8(3)	C(89B)-C(87)-C(88B)	113.8(6)
C(73)-C(72)-C(71)	123.5(2)	C(88)-C(87)-C(88B)	38.8(3)
C(72)-C(73)-C(74)	119.1(2)	C(89)-C(87)-C(88B)	136.0(6)
C(72)-C(73)-C(91)	121.2(2)	C(89B)-C(87)-C(71)	116.9(4)
C(74)-C(73)-C(91)	119.7(2)	C(88)-C(87)-C(71)	114.2(4)
O(4)-C(74)-C(69)	123.2(2)	C(89)-C(87)-C(71)	113.2(4)
O(4)-C(74)-C(73)	119.05(19)	C(88B)-C(87)-C(71)	110.5(5)
C(69)-C(74)-C(73)	117.8(2)	C(89B)-C(87)-C(90)	62.0(4)
C(59)-C(75)-C(77)	113.0(2)	C(88)-C(87)-C(90)	100.0(4)
C(59)-C(75)-C(78)	110.1(2)	C(89)-C(87)-C(90)	100.9(5)
C(77)-C(75)-C(78)	106.8(2)	C(88B)-C(87)-C(90)	63.3(5)
C(59)-C(75)-C(76)	108.82(19)	C(71)-C(87)-C(90)	104.9(4)
C(77)-C(75)-C(76)	106.9(2)	C(89B)-C(87)-C(90B)	111.0(5)
C(78)-C(75)-C(76)	111.2(2)	C(88)-C(87)-C(90B)	56.9(4)
C(80)-C(79)-C(61)	111.4(2)	C(89)-C(87)-C(90B)	76.0(5)
C(80)-C(79)-C(81)	110.8(3)	C(88B)-C(87)-C(90B)	95.4(5)
C(61)-C(79)-C(81)	109.9(2)	C(71)-C(87)-C(90B)	106.9(4)
C(80)-C(79)-C(82)	108.0(3)	C(90)-C(87)-C(90B)	146.4(5)
C(61)-C(79)-C(82)	112.5(3)	C(94)-C(91)-C(93)	110.0(2)
C(81)-C(79)-C(82)	104.1(2)	C(94)-C(91)-C(92)	107.2(2)
C(86)-C(83)-C(84)	116.2(4)	C(93)-C(91)-C(92)	107.0(2)

C(94)-C(91)-C(73)	109.6(2)
C(93)-C(91)-C(73)	111.3(2)
C(92)-C(91)-C(73)	111.6(2)
C(100)-C(95)-C(96)	118.0(3)
C(100)-C(95)-P(2)	123.2(2)
C(96)-C(95)-P(2)	118.9(2)
C(97)-C(96)-C(95)	120.8(3)
C(98)-C(97)-C(96)	119.8(3)
C(99)-C(98)-C(97)	120.1(3)
C(98)-C(99)-C(100)	120.4(3)
C(99)-C(100)-C(95)	120.9(3)
C(102)-C(101)-C(106)	118.7(2)
C(102)-C(101)-P(2)	123.7(2)
C(106)-C(101)-P(2)	117.5(2)
C(101)-C(102)-C(103)	120.6(3)
C(104)-C(103)-C(102)	120.3(3)
C(103)-C(104)-C(105)	119.5(3)
C(104)-C(105)-C(106)	120.5(3)
C(105)-C(106)-C(101)	120.5(3)
C(112)-C(107)-C(108)	119.5(2)
C(112)-C(107)-P(2)	125.8(2)
C(108)-C(107)-P(2)	114.63(19)
C(107)-C(108)-C(109)	119.9(3)
C(110)-C(109)-C(108)	119.8(3)
C(109)-C(110)-C(111)	120.1(2)
C(110)-C(111)-C(112)	120.5(3)
C(107)-C(112)-C(111)	120.2(3)
N(4)-C(113)-C(114)	171.7(2)
C(113)-C(114)-Ir(1)	105.13(16)

Table S69. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **19**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	174(1)	179(1)	149(1)	14(1)	-23(1)	36(1)
Ir(2)	182(1)	193(1)	183(1)	34(1)	-12(1)	45(1)
P(1)	176(4)	212(3)	171(3)	11(2)	-5(3)	46(3)
P(2)	225(4)	243(3)	220(4)	32(3)	-18(3)	83(3)
O(1)	217(10)	220(8)	178(9)	-7(7)	-58(8)	35(7)
O(2)	186(10)	213(8)	158(8)	6(6)	-35(7)	33(7)
O(3)	238(10)	201(8)	219(9)	31(7)	29(8)	37(7)
O(4)	169(10)	222(8)	246(9)	51(7)	-22(8)	32(7)
N(1)	192(12)	164(9)	141(10)	0(7)	-32(8)	43(8)
N(2)	234(13)	217(10)	212(11)	27(8)	-9(9)	89(9)
N(3)	207(12)	201(9)	128(10)	31(8)	-25(9)	38(8)
N(4)	195(12)	206(9)	140(10)	43(8)	7(9)	31(9)
C(1)	264(15)	185(11)	153(12)	15(9)	-79(11)	65(10)
C(2)	330(17)	167(11)	194(13)	20(9)	-81(12)	36(11)
C(3)	418(19)	173(11)	211(14)	-36(10)	-74(13)	46(12)
C(4)	389(18)	193(11)	196(13)	-17(10)	-35(12)	80(12)
C(5)	323(16)	198(11)	167(13)	2(9)	-39(11)	52(11)
C(6)	277(15)	176(10)	126(12)	-5(9)	-59(11)	65(10)
C(7)	210(14)	184(10)	152(12)	-8(9)	-38(10)	60(10)
C(8)	306(16)	201(11)	143(12)	-11(9)	1(11)	80(11)
C(9)	318(16)	186(11)	179(13)	1(9)	25(11)	56(11)
C(10)	303(16)	166(10)	190(13)	-36(9)	5(11)	39(10)
C(11)	193(14)	172(10)	164(12)	-7(9)	-18(10)	66(10)
C(12)	183(14)	227(11)	138(12)	-20(9)	-5(10)	55(10)

C(13)	240(15)	207(11)	175(13)	-6(9)	17(11)	55(10)
C(14)	232(15)	238(11)	196(13)	-44(10)	7(11)	35(11)
C(15)	252(16)	322(13)	142(13)	-56(10)	-7(11)	60(11)
C(16)	187(14)	263(12)	154(12)	-6(9)	-1(10)	67(10)
C(17)	147(13)	233(11)	166(12)	-17(9)	-9(10)	42(10)
C(18)	333(17)	217(12)	266(15)	14(10)	-63(12)	14(11)
C(19)	404(19)	269(13)	339(16)	82(12)	-25(14)	2(13)
C(20)	324(18)	278(13)	336(16)	3(11)	-98(13)	8(12)
C(21)	440(20)	228(12)	428(18)	-59(12)	-50(15)	-35(13)
C(22)	460(20)	232(12)	366(17)	-86(11)	69(15)	85(13)
C(23)	470(30)	850(30)	470(30)	-210(20)	-50(20)	380(30)
C(24)	610(40)	740(30)	410(30)	-330(20)	-10(20)	250(30)
C(25)	1600(80)	440(30)	1130(60)	-120(30)	1130(60)	100(40)
C(26)	510(20)	205(12)	237(15)	-10(10)	127(14)	-10(13)
C(27)	510(20)	470(17)	590(20)	164(16)	278(18)	55(16)
C(28)	760(30)	501(18)	430(20)	267(16)	191(18)	196(18)
C(29)	1320(40)	331(16)	420(20)	-55(14)	330(20)	-330(20)
C(30)	443(19)	245(12)	172(13)	-61(10)	-7(13)	56(12)
C(31)	400(20)	281(13)	353(17)	-31(12)	-36(14)	-26(13)
C(32)	520(20)	284(13)	345(17)	-55(12)	95(15)	128(14)
C(33)	830(30)	280(14)	272(16)	-111(12)	-35(17)	30(16)
C(34)	279(16)	300(12)	149(13)	17(10)	-20(11)	60(12)
C(35)	337(18)	391(14)	205(14)	70(11)	62(12)	93(13)
C(36)	450(20)	387(14)	155(14)	7(11)	-41(13)	88(14)
C(37)	283(16)	350(13)	207(14)	55(11)	-35(12)	90(12)
C(38)	224(15)	308(13)	205(13)	5(10)	1(11)	116(11)
C(39)	250(16)	426(15)	281(16)	35(12)	69(13)	95(13)
C(40)	410(20)	640(20)	326(18)	84(16)	180(15)	148(17)
C(41)	470(20)	660(20)	205(16)	-40(14)	74(15)	198(18)

C(42)	347(19)	449(16)	241(15)	-70(12)	12(13)	160(14)
C(43)	252(16)	351(14)	217(14)	-4(11)	4(12)	141(12)
C(44)	172(14)	295(12)	199(13)	46(10)	-3(11)	45(11)
C(45)	235(15)	284(12)	226(14)	61(10)	-18(11)	56(11)
C(46)	257(16)	308(13)	292(15)	71(11)	-4(12)	-12(12)
C(47)	180(15)	450(16)	286(15)	76(12)	-22(12)	29(13)
C(48)	216(16)	376(15)	380(17)	54(13)	5(13)	98(13)
C(49)	249(16)	313(13)	334(16)	44(12)	26(13)	71(12)
C(50)	173(14)	202(11)	219(13)	9(9)	1(11)	42(10)
C(51)	215(15)	215(11)	216(13)	-19(10)	-24(11)	92(10)
C(52)	262(16)	317(13)	173(13)	26(10)	10(11)	111(12)
C(53)	335(17)	243(12)	303(16)	61(11)	-27(13)	72(12)
C(54)	425(19)	193(12)	337(16)	-13(11)	-13(14)	97(12)
C(55)	291(16)	272(12)	195(13)	-22(10)	5(12)	98(11)
C(56)	153(13)	268(12)	132(12)	37(9)	-7(10)	-5(10)
C(57)	222(15)	200(11)	224(13)	34(10)	6(11)	42(10)
C(58)	264(16)	195(11)	232(14)	85(10)	20(12)	80(11)
C(59)	274(16)	212(11)	258(14)	86(10)	31(12)	49(11)
C(60)	248(16)	275(13)	322(16)	126(12)	55(13)	53(12)
C(61)	310(17)	230(12)	284(15)	112(11)	89(13)	107(12)
C(62)	373(18)	204(11)	228(14)	68(10)	34(12)	107(12)
C(63)	274(16)	200(11)	197(13)	78(10)	31(11)	72(11)
C(64)	284(16)	203(11)	218(13)	40(10)	36(12)	103(11)
C(65)	341(18)	334(13)	213(14)	35(11)	27(12)	151(13)
C(66)	327(18)	449(15)	194(14)	-44(12)	-17(13)	175(14)
C(67)	237(16)	419(15)	263(15)	-44(12)	-59(13)	97(13)
C(68)	222(15)	258(12)	248(14)	16(10)	-23(12)	105(11)
C(69)	215(15)	302(13)	258(14)	10(11)	-25(12)	74(11)
C(70)	248(17)	526(17)	250(15)	53(13)	-41(13)	112(14)

C(71)	185(17)	660(20)	326(17)	41(15)	-37(13)	62(15)
C(72)	208(16)	446(16)	349(17)	39(13)	-5(13)	-20(13)
C(73)	204(15)	316(13)	287(15)	39(11)	4(12)	31(11)
C(74)	208(15)	259(12)	256(14)	10(10)	-18(12)	53(11)
C(75)	258(16)	341(14)	278(15)	46(12)	32(12)	-19(12)
C(76)	301(18)	453(16)	301(16)	62(13)	-4(13)	44(14)
C(77)	370(20)	525(18)	460(20)	-43(15)	46(16)	-117(16)
C(78)	460(20)	278(13)	306(16)	18(11)	88(14)	-13(13)
C(79)	334(18)	303(13)	393(17)	63(12)	129(14)	108(13)
C(80)	1060(40)	1550(40)	590(30)	230(30)	170(30)	1050(40)
C(81)	680(30)	640(20)	520(20)	133(18)	310(20)	210(20)
C(82)	700(30)	550(20)	750(30)	-132(19)	350(20)	50(20)
C(83)	400(20)	980(30)	221(17)	-68(17)	-54(15)	250(20)
C(84)	790(40)	1720(50)	400(20)	-450(30)	-60(20)	400(30)
C(85)	710(30)	1130(30)	440(20)	310(20)	-40(20)	160(30)
C(86)	470(30)	1910(50)	310(20)	200(30)	-97(19)	20(30)
C(87)	240(20)	1380(40)	360(20)	140(20)	-41(16)	160(20)
C(91)	219(16)	355(14)	359(17)	112(13)	2(13)	22(12)
C(92)	270(18)	510(18)	570(20)	224(16)	96(15)	38(15)
C(93)	341(18)	449(16)	303(16)	136(13)	24(14)	96(14)
C(94)	293(17)	314(14)	440(18)	115(13)	46(14)	52(13)
C(95)	281(17)	338(14)	295(16)	70(12)	37(13)	148(13)
C(96)	348(19)	488(17)	344(17)	101(14)	42(15)	160(15)
C(97)	540(30)	740(20)	326(19)	141(17)	135(17)	220(20)
C(98)	460(20)	760(20)	590(30)	240(20)	240(20)	200(20)
C(99)	320(20)	590(20)	570(20)	166(18)	134(17)	136(16)
C(100)	303(18)	386(15)	427(18)	100(13)	46(15)	139(14)
C(101)	302(17)	270(12)	181(13)	6(10)	-20(12)	103(12)
C(102)	339(17)	265(12)	217(14)	50(10)	24(12)	82(12)

C(103)	335(18)	339(14)	213(14)	8(11)	-24(13)	44(13)
C(104)	520(20)	342(14)	211(15)	-56(11)	-27(14)	73(15)
C(105)	500(20)	361(15)	309(16)	-79(12)	-8(15)	201(15)
C(106)	351(19)	373(15)	285(16)	-56(12)	-64(13)	148(14)
C(107)	280(16)	234(12)	210(13)	-8(10)	-47(12)	81(11)
C(108)	281(16)	208(11)	277(15)	-1(10)	-49(12)	84(11)
C(109)	460(20)	216(12)	213(14)	-38(10)	-34(13)	64(12)
C(110)	380(20)	323(14)	321(16)	38(12)	-153(14)	73(13)
C(111)	297(19)	466(17)	510(20)	115(15)	-147(16)	85(14)
C(112)	289(17)	355(14)	343(16)	85(12)	0(13)	116(13)
C(113)	222(15)	207(11)	146(12)	23(9)	25(11)	-14(10)
C(114)	192(14)	258(12)	211(13)	32(10)	-22(11)	60(10)

$(ONO^{tBu})Ir(PEt_3)_2Cl$

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S70. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **$(ONO^{tBu})Ir(PEt_3)_2Cl$**. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	9002(1)	952(1)	2905(1)	13(1)

P(1)	9090(1)	934(1)	824(1)	15(1)
P(2)	8952(1)	890(1)	4978(1)	15(1)
Cl(1)	9778(1)	336(1)	2899(1)	18(1)
O(1)	10539(1)	1186(1)	2862(1)	15(1)
O(2)	7461(1)	723(1)	2934(1)	14(1)
N(1)	8361(1)	1480(1)	2918(1)	12(1)
C(1)	10812(1)	1456(1)	3618(1)	14(1)
C(2)	11935(1)	1504(1)	4025(1)	17(1)
C(3)	12168(1)	1746(1)	4961(1)	18(1)
C(4)	11383(1)	1963(1)	5508(1)	16(1)
C(5)	10332(1)	1951(1)	4993(1)	15(1)
C(6)	10036(1)	1713(1)	4035(1)	14(1)
C(7)	8945(1)	1771(1)	3437(1)	13(1)
C(8)	8526(1)	2136(1)	3386(1)	14(1)
C(9)	7477(1)	2212(1)	2908(1)	14(1)
C(10)	6888(1)	1907(1)	2448(1)	14(1)
C(11)	7345(1)	1546(1)	2411(1)	12(1)
C(12)	6683(1)	1244(1)	1827(1)	13(1)
C(13)	5954(1)	1354(1)	884(1)	14(1)
C(14)	5182(1)	1114(1)	364(1)	15(1)
C(15)	5092(1)	758(1)	889(1)	16(1)
C(16)	5787(1)	627(1)	1808(1)	14(1)
C(17)	6678(1)	864(1)	2214(1)	13(1)
C(18)	12847(1)	1307(1)	3388(2)	21(1)
C(19)	12745(1)	874(1)	3374(2)	27(1)
C(20)	13993(1)	1403(1)	3934(2)	33(1)
C(21)	12800(1)	1457(1)	2113(2)	26(1)
C(22)	11662(1)	2187(1)	6642(1)	18(1)
C(23)	11380(2)	1942(1)	7692(2)	29(1)

C(24)	12877(1)	2295(1)	6767(2)	26(1)
C(25)	11010(2)	2556(1)	6673(2)	29(1)
C(26)	7033(1)	2615(1)	2913(1)	15(1)
C(27)	7771(1)	2873(1)	2222(2)	24(1)
C(28)	7036(1)	2755(1)	4190(2)	22(1)
C(29)	5866(1)	2643(1)	2363(2)	21(1)
C(30)	4506(1)	1237(1)	-750(1)	19(1)
C(31)	5201(2)	1176(1)	-1815(2)	32(1)
C(32)	3446(1)	1010(1)	-926(2)	26(1)
C(33)	4189(1)	1656(1)	-696(2)	24(1)
C(34)	5624(1)	238(1)	2376(1)	17(1)
C(35)	4588(1)	38(1)	1863(2)	22(1)
C(36)	6598(1)	-24(1)	2187(2)	22(1)
C(37)	5494(1)	287(1)	3700(1)	21(1)
C(38)	8141(1)	624(1)	-42(1)	19(1)
C(39)	8443(1)	204(1)	-32(2)	24(1)
C(40)	10445(1)	778(1)	429(1)	18(1)
C(41)	10642(1)	780(1)	-880(1)	23(1)
C(42)	8891(1)	1381(1)	26(1)	20(1)
C(43)	9730(1)	1683(1)	368(2)	25(1)
C(44)	8435(1)	423(1)	5355(1)	19(1)
C(45)	8136(1)	366(1)	6626(2)	24(1)
C(46)	10210(1)	941(1)	5921(1)	21(1)
C(47)	11041(1)	626(1)	5812(2)	28(1)
C(48)	8059(1)	1226(1)	5695(1)	20(1)
C(49)	6843(1)	1207(1)	5303(2)	24(1)

Table S71. Selected bond lengths [Å] and angles [°] for **(ONO^{tBu})Ir(PEt$_3$)$_2$Cl**.

Ir(1)-N(1)	2.0305(11)	N(1)-Ir(1)-O(2)	90.35(4)
Ir(1)-O(2)	2.0581(10)	N(1)-Ir(1)-O(1)	89.11(4)
Ir(1)-O(1)	2.0623(10)	O(2)-Ir(1)-O(1)	179.31(4)
Ir(1)-P(2)	2.3735(4)	N(1)-Ir(1)-P(2)	92.53(3)
Ir(1)-P(1)	2.3763(4)	O(2)-Ir(1)-P(2)	82.53(3)
Ir(1)-Cl(1)	2.3792(4)	O(1)-Ir(1)-P(2)	97.91(3)
		N(1)-Ir(1)-P(1)	94.17(3)
		O(2)-Ir(1)-P(1)	95.79(3)
		O(1)-Ir(1)-P(1)	83.83(3)
		P(2)-Ir(1)-P(1)	173.104(13)
		N(1)-Ir(1)-Cl(1)	179.21(3)
		O(2)-Ir(1)-Cl(1)	90.38(3)
		O(1)-Ir(1)-Cl(1)	90.17(3)
		P(2)-Ir(1)-Cl(1)	87.267(13)
		P(1)-Ir(1)-Cl(1)	86.053(13)

Table S72. Bond lengths [Å] and angles [°] for **(ONO^{tBu})Ir(PEt$_3$)$_2$Cl**.

Ir(1)-N(1)	2.0305(11)	C(9)-C(10)	1.3851(19)
Ir(1)-O(2)	2.0581(10)	C(9)-C(26)	1.5277(19)
Ir(1)-O(1)	2.0623(10)	C(10)-C(11)	1.3992(19)
Ir(1)-P(2)	2.3735(4)	C(11)-C(12)	1.4787(19)
Ir(1)-P(1)	2.3763(4)	C(12)-C(13)	1.4109(19)
Ir(1)-Cl(1)	2.3792(4)	C(12)-C(17)	1.4162(19)
P(1)-C(40)	1.8327(15)	C(13)-C(14)	1.3782(19)
P(1)-C(42)	1.8354(15)	C(14)-C(15)	1.406(2)
P(1)-C(38)	1.8431(15)	C(14)-C(30)	1.536(2)
P(2)-C(44)	1.8327(16)	C(15)-C(16)	1.389(2)
P(2)-C(46)	1.8357(15)	C(16)-C(17)	1.434(2)
P(2)-C(48)	1.8404(15)	C(16)-C(34)	1.538(2)
O(1)-C(1)	1.3179(17)	C(18)-C(20)	1.541(2)
O(2)-C(17)	1.3232(16)	C(18)-C(21)	1.542(2)
N(1)-C(7)	1.3689(17)	C(18)-C(19)	1.540(2)
N(1)-C(11)	1.3617(17)	C(22)-C(25)	1.531(2)
C(1)-C(6)	1.4177(19)	C(22)-C(24)	1.537(2)
C(1)-C(2)	1.4364(19)	C(22)-C(23)	1.534(2)
C(2)-C(3)	1.384(2)	C(26)-C(29)	1.532(2)
C(2)-C(18)	1.535(2)	C(26)-C(28)	1.536(2)
C(3)-C(4)	1.406(2)	C(26)-C(27)	1.534(2)
C(4)-C(5)	1.3845(19)	C(30)-C(32)	1.532(2)
C(4)-C(22)	1.537(2)	C(30)-C(33)	1.536(2)
C(5)-C(6)	1.410(2)	C(30)-C(31)	1.537(2)
C(6)-C(7)	1.4790(19)	C(34)-C(35)	1.540(2)
C(7)-C(8)	1.3918(19)	C(34)-C(37)	1.534(2)
C(8)-C(9)	1.3939(19)	C(34)-C(36)	1.539(2)

C(38)-C(39)	1.531(2)	C(44)-P(2)-C(48)	104.95(7)
C(40)-C(41)	1.522(2)	C(46)-P(2)-C(48)	100.31(8)
C(42)-C(43)	1.520(2)	C(44)-P(2)-Ir(1)	110.17(5)
C(44)-C(45)	1.526(2)	C(46)-P(2)-Ir(1)	120.09(6)
C(46)-C(47)	1.522(2)	C(48)-P(2)-Ir(1)	115.59(5)
C(48)-C(49)	1.532(2)	C(1)-O(1)-Ir(1)	118.34(9)
		C(17)-O(2)-Ir(1)	118.38(9)
N(1)-Ir(1)-O(2)	90.35(4)	C(7)-N(1)-C(11)	119.70(11)
N(1)-Ir(1)-O(1)	89.11(4)	C(7)-N(1)-Ir(1)	120.24(9)
O(2)-Ir(1)-O(1)	179.31(4)	C(11)-N(1)-Ir(1)	120.06(9)
N(1)-Ir(1)-P(2)	92.53(3)	O(1)-C(1)-C(6)	122.33(12)
O(2)-Ir(1)-P(2)	82.53(3)	O(1)-C(1)-C(2)	119.81(12)
O(1)-Ir(1)-P(2)	97.91(3)	C(6)-C(1)-C(2)	117.84(13)
N(1)-Ir(1)-P(1)	94.17(3)	C(3)-C(2)-C(1)	118.11(13)
O(2)-Ir(1)-P(1)	95.79(3)	C(3)-C(2)-C(18)	121.39(13)
O(1)-Ir(1)-P(1)	83.83(3)	C(1)-C(2)-C(18)	120.40(13)
P(2)-Ir(1)-P(1)	173.104(13)	C(2)-C(3)-C(4)	124.31(13)
N(1)-Ir(1)-Cl(1)	179.21(3)	C(5)-C(4)-C(3)	116.17(13)
O(2)-Ir(1)-Cl(1)	90.38(3)	C(5)-C(4)-C(22)	121.80(13)
O(1)-Ir(1)-Cl(1)	90.17(3)	C(3)-C(4)-C(22)	121.99(13)
P(2)-Ir(1)-Cl(1)	87.267(13)	C(4)-C(5)-C(6)	122.42(13)
P(1)-Ir(1)-Cl(1)	86.053(13)	C(5)-C(6)-C(1)	119.72(12)
C(40)-P(1)-C(42)	103.58(7)	C(5)-C(6)-C(7)	117.24(12)
C(40)-P(1)-C(38)	104.03(7)	C(1)-C(6)-C(7)	122.76(13)
C(42)-P(1)-C(38)	100.87(7)	N(1)-C(7)-C(8)	119.94(12)
C(40)-P(1)-Ir(1)	110.32(5)	N(1)-C(7)-C(6)	122.04(12)
C(42)-P(1)-Ir(1)	117.18(6)	C(8)-C(7)-C(6)	118.01(12)
C(38)-P(1)-Ir(1)	119.00(5)	C(7)-C(8)-C(9)	121.81(13)
C(44)-P(2)-C(46)	104.07(7)	C(10)-C(9)-C(8)	116.40(13)

C(10)-C(9)-C(26)	123.50(12)	C(4)-C(22)-C(23)	108.07(13)
C(8)-C(9)-C(26)	120.09(12)	C(25)-C(22)-C(23)	108.87(15)
C(9)-C(10)-C(11)	121.58(13)	C(24)-C(22)-C(23)	109.32(13)
N(1)-C(11)-C(10)	120.22(12)	C(29)-C(26)-C(9)	112.53(12)
N(1)-C(11)-C(12)	122.01(12)	C(29)-C(26)-C(28)	108.42(12)
C(10)-C(11)-C(12)	117.76(12)	C(9)-C(26)-C(28)	108.90(12)
C(13)-C(12)-C(17)	119.05(12)	C(29)-C(26)-C(27)	108.53(13)
C(13)-C(12)-C(11)	116.62(12)	C(9)-C(26)-C(27)	109.48(12)
C(17)-C(12)-C(11)	124.14(12)	C(28)-C(26)-C(27)	108.93(13)
C(14)-C(13)-C(12)	122.96(13)	C(32)-C(30)-C(33)	107.29(13)
C(13)-C(14)-C(15)	116.18(13)	C(32)-C(30)-C(14)	111.84(13)
C(13)-C(14)-C(30)	120.23(13)	C(33)-C(30)-C(14)	111.44(13)
C(15)-C(14)-C(30)	123.55(13)	C(32)-C(30)-C(31)	109.17(14)
C(16)-C(15)-C(14)	124.04(13)	C(33)-C(30)-C(31)	108.79(14)
C(15)-C(16)-C(17)	117.98(13)	C(14)-C(30)-C(31)	108.27(13)
C(15)-C(16)-C(34)	121.71(13)	C(16)-C(34)-C(35)	112.23(12)
C(17)-C(16)-C(34)	120.30(13)	C(16)-C(34)-C(37)	109.57(12)
O(2)-C(17)-C(12)	122.34(12)	C(35)-C(34)-C(37)	107.08(13)
O(2)-C(17)-C(16)	119.36(12)	C(16)-C(34)-C(36)	111.13(12)
C(12)-C(17)-C(16)	118.31(12)	C(35)-C(34)-C(36)	107.33(13)
C(20)-C(18)-C(21)	106.65(15)	C(37)-C(34)-C(36)	109.36(13)
C(20)-C(18)-C(19)	107.21(14)	C(39)-C(38)-P(1)	115.41(11)
C(21)-C(18)-C(19)	109.50(14)	C(41)-C(40)-P(1)	115.86(11)
C(20)-C(18)-C(2)	112.46(13)	C(43)-C(42)-P(1)	114.44(11)
C(21)-C(18)-C(2)	107.53(13)	C(45)-C(44)-P(2)	116.56(12)
C(19)-C(18)-C(2)	113.27(14)	C(47)-C(46)-P(2)	115.09(12)
C(4)-C(22)-C(25)	111.67(12)	C(49)-C(48)-P(2)	115.92(11)
C(4)-C(22)-C(24)	111.95(13)		
C(25)-C(22)-C(24)	106.91(14)		

Table S73. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **(ONO^{tBu})Ir(PEt$_3$)$_2$Cl**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	128(1)	113(1)	133(1)	0(1)	-6(1)	21(1)
P(1)	152(2)	157(2)	137(2)	-6(1)	3(1)	8(1)
P(2)	172(2)	144(2)	136(2)	3(1)	-4(1)	19(1)
Cl(1)	221(2)	153(1)	177(2)	7(1)	7(1)	50(1)
O(1)	109(4)	165(5)	187(5)	-42(4)	0(3)	-3(3)
O(2)	119(4)	133(4)	177(5)	26(4)	-13(3)	-9(3)
N(1)	124(5)	94(4)	147(5)	1(4)	-4(4)	18(4)
C(1)	125(6)	151(6)	143(6)	-2(4)	-5(4)	8(4)
C(2)	135(6)	198(7)	187(7)	-18(5)	-5(5)	21(5)
C(3)	128(6)	223(7)	198(7)	-27(5)	-28(5)	13(5)
C(4)	138(6)	160(6)	163(6)	-12(5)	-21(4)	6(5)
C(5)	133(6)	148(6)	161(6)	-7(5)	-9(4)	12(4)
C(6)	117(5)	139(6)	155(6)	3(4)	-8(4)	18(4)
C(7)	129(5)	117(5)	141(6)	-2(4)	-3(4)	7(4)
C(8)	135(6)	125(5)	167(6)	-4(4)	-16(4)	6(4)
C(9)	142(6)	122(5)	146(6)	5(4)	-2(4)	12(4)
C(10)	131(6)	131(6)	162(6)	1(4)	-20(4)	10(4)
C(11)	125(5)	111(5)	137(6)	11(4)	-8(4)	13(4)
C(12)	134(6)	121(5)	140(6)	4(4)	-3(4)	2(4)
C(13)	145(6)	125(5)	154(6)	12(4)	-10(4)	0(4)
C(14)	144(6)	152(6)	148(6)	4(5)	-8(4)	-10(5)
C(15)	148(6)	154(6)	176(7)	0(5)	2(5)	-20(5)
C(16)	154(6)	132(6)	150(6)	0(4)	16(4)	-4(5)
C(17)	130(5)	130(5)	129(6)	7(4)	4(4)	8(4)

C(18)	137(6)	275(8)	218(8)	-57(6)	-6(5)	45(5)
C(19)	202(8)	250(8)	356(10)	-23(7)	11(7)	72(6)
C(20)	142(7)	453(12)	388(11)	-153(9)	-8(7)	43(7)
C(21)	208(8)	315(9)	269(9)	-30(7)	69(6)	2(6)
C(22)	158(6)	213(7)	176(7)	-34(5)	-36(5)	9(5)
C(23)	289(9)	379(10)	192(8)	-8(7)	-9(6)	-49(8)
C(24)	194(7)	308(9)	258(9)	-62(7)	-43(6)	-34(6)
C(25)	264(9)	281(9)	305(9)	-114(7)	-71(7)	57(7)
C(26)	157(6)	123(5)	177(6)	-9(5)	-12(5)	24(5)
C(27)	250(8)	157(6)	302(9)	52(6)	26(6)	9(6)
C(28)	238(8)	210(7)	220(8)	-53(6)	-19(6)	56(6)
C(29)	196(7)	179(7)	254(8)	-29(5)	-45(5)	59(5)
C(30)	185(7)	192(7)	178(7)	11(5)	-44(5)	-17(5)
C(31)	360(10)	400(11)	184(8)	30(7)	3(7)	5(8)
C(32)	266(8)	234(8)	263(9)	16(6)	-118(6)	-64(6)
C(33)	240(8)	213(7)	260(8)	59(6)	-88(6)	-15(6)
C(34)	193(7)	132(6)	186(7)	15(5)	22(5)	-12(5)
C(35)	243(8)	173(7)	255(8)	13(6)	14(6)	-61(6)
C(36)	245(8)	145(6)	286(9)	1(6)	38(6)	2(6)
C(37)	230(7)	213(7)	191(7)	41(6)	37(5)	2(6)
C(38)	171(6)	238(7)	166(7)	-52(5)	-5(5)	-5(5)
C(39)	244(8)	225(8)	247(8)	-45(6)	8(6)	-47(6)
C(40)	149(6)	212(7)	165(7)	-23(5)	6(5)	7(5)
C(41)	196(7)	305(9)	188(7)	-31(6)	30(5)	-28(6)
C(42)	216(7)	201(7)	172(7)	46(5)	10(5)	15(5)
C(43)	299(9)	202(7)	240(8)	31(6)	25(6)	-28(6)
C(44)	213(7)	188(7)	169(7)	25(5)	-2(5)	-5(5)
C(45)	278(8)	244(8)	216(8)	54(6)	44(6)	17(6)
C(46)	239(7)	220(7)	157(6)	22(6)	-41(5)	-5(6)

C(47)	233(8)	287(9)	316(10)	24(7)	-46(7)	37(7)
C(48)	238(7)	200(7)	154(7)	-23(5)	39(5)	23(6)
C(49)	229(8)	274(8)	229(8)	-16(6)	29(6)	57(6)

VII. Cyclic Voltammetry

Cyclic voltammetry was carried out in the air at room temperature. The solvent was dichloromethane with 0.1 M tetrabutylammonium tetrafluoroborate added as the electrolyte. Multiple runs were made with scan rates from 50 to 400 mV/s. Quasireversibility is seen in the form of a following chemical step.

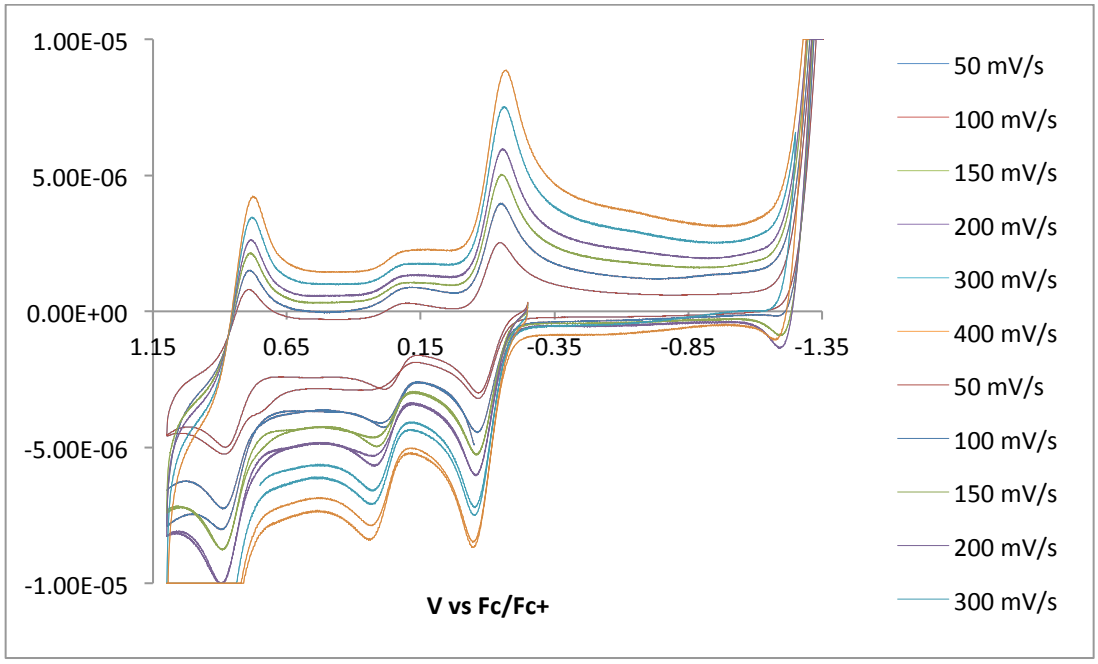


Figure S24. Cyclic voltammetry of (ONO^{tBu})Ir(PEt$_3$)$_2$Me, **14**. The dip at 0.3 V is an artifact.

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